# Construction and Optimization Techniques for High Order Schemes for the Two-dimensional Wave Equation

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*To be presented at the 21st International Congress on Acoustics, Montréal, Canada, 2013*

**Abstract**

With the advent of high performance parallel computing, audio rate room auralization using finite difference time domain methods is becoming possible in a reasonable computation time. Yet, there are still deficiencies in the methods which are used for this purpose, particularly with regard to minimizing numerical dispersion over the full range of audible frequencies.

This paper is concerned with construction techniques for families of methods for the test case of the 2D wave equation. Such methods are explicit, can be of very high accuracy, and operate over a small local stencil. Such schemes can be attractive in a parallel computation environment. As such methods will depend, invariably, on a set of free parameters, including the Courant number, a major concern is optimization. The remainder of this paper approaches the problem of setting up such an optimization problem in terms of various constraints and a suitable cost function. Some of the constraints follow from consistency, stability, isotropy and accuracy of the resulting scheme, and others from perceptual considerations peculiar to audio.

Simulation results will be presented.

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## INTRODUCTION

Room acoustics simulation, for purposes of room auralization, or artificial reverberation, can be carried out in a variety of ways. Many techniques currently in use are based on ray tracing [1] or image source methods [2]—while efficient algorithms are available in these cases, allowing for rendering in a reasonable amount of time, these methods do possess certain weaknesses—ray tracing methods are a good approximation at high frequencies, and image source methods can become very complex, computationally, when the domain of interest is no longer of a geometrically simple form.

Finite difference time domain (FDTD) methods [3, 4], while computationally much more costly, allow a complete rendering of the entire acoustic field within an enclosure—in theory! In practice, however, FDTD methods can introduce audible artifacts of their own, and particularly spurious numerical dispersion, leading to wave propagation at speeds which are frequency and direction dependent. One remedy to this problem is to operate at an oversampled rate—but, for all FDTD simulations, the memory requirements/operation count scale as a power of the sample rate, and thus there is a premium on algorithms which operate at an audio rate (such as 44.1 kHz, 48 kHz, etc.).

Another approach is design more complex schemes, for which updates depend on not just nearest neighbour points, either targeting numerical anisotropy or dispersion as a whole. While such schemes require more arithmetic operations, the memory requirement is not significantly altered—such algorithms are well suited to implementation in parallel hardware [5]. The design problem, however, becomes significantly more complex, as one is faced with a parameterized FDTD method, where the number of parameters may be quite large. There are two difficulties here: determining sufficient conditions for numerical stability for such methods, and finding a means of optimizing such schemes to target the minimization of numerical dispersion (while bearing in mind various constaints peculiar to audio which play an important role in setting up the resulting optimization problem).

In this article, for simplicity, the system of interest is the wave equation in 2D. The modified equation method [6, 7] is applied to schemes dependent on a number of free parameters, in order to arrive at families of schemes of a specified order of isotropy and accuracy. Such specifications can then be used in order to set up an optimization problem, the solution of which can be approached in a variety of ways. Simulation results are presented, comparing modified equation approaches to accuracy with global minimization of phase velocity error over wavenumber space.

## APPROXIMATIONS TO THE LAPLACIAN OVER A REGULAR GRID

Consider the Laplacian operator in 2D, defined, in Cartesian coordinates, as

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \tag{1}$$

In this section, approximations to the Laplacian over a regular grid, of spacing $h$ are considered. Over such a grid, a grid function $u_{\xi_x,\xi_y}$, depending on two grid indeces $\xi_x$ and $\xi_y$ is intended as an approximation to some underlying function $u(x,y)$, at locations $x = \xi_x h$ and $y = \xi_y h$.

Over such a grid, a symmetric approximation $\hat{\delta}_{l,m}$ to the Laplacian operator $\nabla^2$, including grid points distant from the operating point by $(l,m)$ or $(m,l)$ units may be written as

$$\hat{\delta}_{l,m} = \frac{2}{h^2\left(l^2+m^2\right)}\left(\mu_{l,x}\mu_{m,y} + \mu_{m,x}\mu_{l,y} - 2\right) = \nabla^2 + O(h^2) \tag{2}$$

where $\mu_{b,x}$ and $\mu_{b,y}$ are averaging operators, defined, for integer $b \geq 0$, in terms of operation over a grid function $u_{\xi_x,\xi_y}$ as

$$\mu_{b,x} u_{\xi_x,\xi_y} = \frac{1}{2}\left(u_{\xi_x+b,\xi_y} + u_{\xi_x-b,\xi_y}\right) \qquad \mu_{b,y} u_{\xi_x,\xi_y} = \frac{1}{2}\left(u_{\xi_x,\xi_y+b} + u_{xi_x,\xi_y-b}\right) \tag{3}$$

The above operators are characterized by integers $l,m$, where, without loss of generality one may choose $l \geq m \geq 0$, and where at least one of $l$, $m$ is nonzero. (Note that the simple five point Laplacian operator corresponds to a choice of $l = 1$, $m = 0$.) Notice also that each such operator selects a distinct family of points surrounding the point of operation, or stencil, allowing a simple computational cost to be associated with each such operator independently of others which may be applied simultaneously (one multiplication, and either four additions (when $l = m$) or eight (when $l \neq m$). See Figure 1, showing the stencils of certain members of this family.

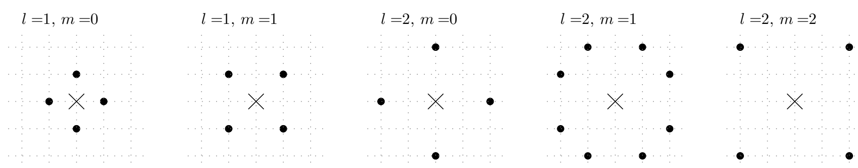


**FIGURE 1:** Stencils of approximations $\hat{\delta}_{l,m}$ to the Laplacian, for various values of $l$, $m$, operating at points marked with a $\times$.

## Spatial Frequency Domain

When applied to a wave-like solution,

$$u_{\xi_x,\xi_y} = e^{jh(\beta_x\xi_x+\beta_y\xi_y)} \tag{4}$$

for wavenumber $\underline{\beta} = [\beta_x, \beta_y]$, the operators $\delta_{l,m}$ behave as multiplicative factors $\delta_{l,m}$:

$$\delta_{l,m} = \frac{2}{h^2\left(l^2+m^2\right)}\left(c_{l,x}c_{m,y} + c_{m,x}c_{l,y} - 2\right) \tag{5}$$

where, for integer $b \geq 0$

$$c_{b,x} = \cos(b\beta_x h) \qquad c_{b,y} = \cos(b\beta_y h) \tag{6}$$

## Series Expansions

Given that one may expand $c_{b,x}$ as

$$c_{b,x} = \sum_{p=0}^{\infty} \frac{(-1)^p}{(2p)!} h^{2p} \beta_x^{2p} \tag{7}$$

and similarly for $c_{b,y}$, one may expand the expression for $\delta_{l,m}$ as

$$\delta_{l,m} = \frac{2}{(l^2+m^2)h^2}\left(\sum_{p=0}^{\infty}\sum_{q=0}^{\infty} \frac{(-1)^{p+q} h^{2(p+q)}}{(2p)!(2q)!}\left(l^{2p}m^{2q} + l^{2q}m^{2p}\right)\beta_x^{2p}\beta_y^{2q} - 2\right) \tag{8}$$

Defining $M$ as

$$M = p + q \tag{9}$$

this expression may be written as

$$\delta_{l,m} = -|\underline{\beta}|^2 + \frac{2}{l^2+m^2}\left(\sum_{M=2}^{\infty}(-1)^M h^{2M-2}\sum_{q=0}^{M}\frac{l^{2(M-q)}m^{2q}+l^{2q}m^{2(M-q)}}{(2q)!(2(M-q))!}\beta_x^{2(M-q)}\beta_y^{2q}\right) \tag{10}$$

or, more compactly, as

$$\delta_{l,m} = -|\underline{\beta}|^2 + 2\left(\sum_{M=2}^{\infty}\frac{(-1)^M h^{2M-2}}{(2M)!}\sum_{q=0}^{M} g_{l,m,M,q}\beta_x^{2(M-q)}\beta_y^{2q}\right) \qquad g_{l,m,M,q} = \frac{(2M)!\left(l^{2(M-q)}m^{2q}+l^{2q}m^{2(M-q)}\right)}{(l^2+m^2)(2q)!(2(M-q))!} \tag{11}$$

## Parameterized Approximations

Consider now a set $\mathscr{Q} = \{(l_1,m_1),(l_2,m_2),\ldots,(l_{N_\mathscr{Q}},m_{N_\mathscr{Q}})\}$ of $N_\mathscr{Q}$ approximations to the Laplacian. The approximation

$$\hat{\delta}_\mathscr{Q} = \sum_{(l,m)\in\mathscr{Q}} \alpha_{l,m}\hat{\delta}_{l,m} \tag{12}$$

is also an approximation to the Laplacian provided that the constants $\alpha_{l,m}$ satisfy the constraint

$$\sum_{(l,m)\in\mathscr{Q}} \alpha_{l,m} = 1 \qquad \textbf{Consistency} \tag{13}$$

For simplicity, the ensemble of such parameters may be written as the vector $\underline{\alpha}$.

The parameterized operator above transforms to

$$\delta_\mathscr{Q} = -|\underline{\beta}|^2 + 2\left(\sum_{M=2}^{\infty}\frac{(-1)^M h^{2M-2}}{(2M)!}\sum_{(l,m)\in\mathscr{Q}}\alpha_{l,m}\sum_{q=0}^{M} g_{l,m,M,q}\beta_x^{2(M-q)}\beta_y^{2q}\right) \tag{14}$$

## Isotropy

The $b$th power of the operator $\nabla^2$ transforms to

$$(-1)^b\,|\underline{\beta}|^{2b} = (-1)^b\left(\beta_x^2+\beta_y^2\right)^b = (-1)^b\sum_{q=0}^{b}\frac{b!}{q!(b-q)!}\beta_x^{2(b-q)}\beta_y^{2q} \tag{15}$$

Suppose that we would like the operator $\delta_\mathscr{Q}$ to be isotropic to $2M_i$th order, where $M_i \geq 2$. This then implies the following linear constraints on $\alpha_{l,m}$:

$$\sum_{(l,m)\in\mathscr{Q}} \alpha_{l,m}g_{l,m,M,q} = r_M\frac{M!}{q!(M-q)!}, \qquad M = 2,\ldots,M_i \qquad q = 0,\ldots,M \tag{16}$$

for some constants $r_M$, $M = 2,\ldots,M_i$. By symmetry, and using $r_M = \sum_{(l,m)\in\mathscr{Q}}\alpha_{l,m}g_{l,m,M,0}$, these can be reduced to the following:

$$\sum_{(l,m)\in\mathscr{Q}} \alpha_{l,m}\left(g_{l,m,M,q} - \frac{M!g_{l,m,M,0}}{q!(M-q)!}\right) = 0, \qquad M = 2,\ldots,M_i \qquad q = 1,\ldots,\mathrm{floor}\left(\frac{M}{2}\right) \qquad \textbf{Isotropy} \tag{17}$$

The transformed operator $\delta_\mathscr{Q}$ may then be written as

$$\delta_\mathscr{Q} = -|\underline{\beta}|^2 + 2\left(\sum_{M=2}^{M_i}\frac{(-1)^M h^{2M-2}}{(2M)!}r_M|\underline{\beta}|^{2M}\right) + O(h^{2M_i}) \tag{18}$$

## TIME DEPENDENT FINITE DIFFERENCE SCHEMES FOR THE WAVE EQUATION

As a simple test case to be discussed in this article, consider the 2D wave equation:

$$\frac{\partial^2 u}{\partial t^2} = \nabla^2 u \qquad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \tag{19}$$

where here, $u = u(x,y,t)$ is a neutral variable, which could signify a pressure distribution, or a velocity potential [8] in an enclosure, at time $t$, and at coordinates $x$ and $y$. For simplicity here, the wave speed has been chosen as 1 (or the system nondimensionalized).

### Two Step Parameterized Schemes

Suppose now that the solution $u(x,y,t)$ is to be approximated by a finite difference scheme, operating with a time step $k$ (where $F_s = 1/k$ is the sample rate). $u^n_{\xi_x,\xi_y}$ represents an approximation to $u(x,y,t)$ at $x = \xi_x h,\ y = \xi_y h,\ t = nk$.

Consider the following two step parameterized scheme:

$$\delta_{tt} u = \delta_{\mathcal{Q}} u \tag{20}$$

for grid function $u^n_{\xi_x,\xi_y}$, where

$$\delta_{tt} u^n_{\xi_x,\xi_y} = \frac{1}{k^2}\left(u^{n+1}_{\xi_x,\xi_y} - 2u^n_{\xi_x,\xi_y} + u^{n-1}_{\xi_x,\xi_y}\right) \tag{21}$$

Here, $\delta_{\mathcal{Q}}$ is some parameterized approximation to the Laplacian operator. Two step schemes are of interest for various reasons in acoustics applications: compared with multistep schemes (such as, e.g., Runge Kutta, Adams Moulton, etc.), such schemes do not introduce spurious parasitic solutions, as the order of the approximation matches that of the model system (here, two). Another benefit, especially important if such schemes are to be used in large room acoustics problem is that of the memory requirement, a critical concern on current parallel hardware, for example—memory requirements grow with the number of steps required in the update, and the two step scheme is minimal in this regard.

Such schemes are also explicit, i.e., the solution may be advanced as

$$u^{n+1} = 2u^n - u^{n-1} + k^2 \delta_{\mathcal{Q}} u^n \tag{22}$$

and thus, compared with implicit methods, requiring linear system solutions (potentially very large in room applications), computational complexity is quite low.

### Modified Equations and Accuracy

For time harmonic grid functions $u^n_{\xi_x,\xi_y} = e^{j(k\omega n + h\beta_x\xi_x + h\beta_y\xi_y)}$, the operator $\delta_{tt}$ becomes a multiplicative factor

$$\frac{-4}{k^2}\sin(\omega k/2) = -\omega^2 + \sum_{M=2}^{M_i} \frac{2(-1)^M k^{2M-2}}{(2M)!}\omega^{2M} + O(k^{2M_i}) \tag{23}$$

Supposing that the approximation $\delta_{\mathcal{Q}}$ is isotropic to $2M_i$th order, the scheme tranforms, as a whole, to

$$-\omega^2 + |\underline{\beta}|^2 + 2\sum_{M=2}^{M_i} \frac{(-1)^M}{(2M)!}\left(k^{2M-2}\omega^{2M} - h^{2M-2} r_M |\underline{\beta}|^{2M}\right) = O(k^{2M_i}, h^{2M_i}) \tag{24}$$

Under the further conditions that

$$r_M = \lambda^{2M-2} \qquad M = 2,\dots,M_i \qquad \text{or} \qquad \sum_{(l,m)\in\mathcal{Q}} \alpha_{l,m} g_{l,m,M,0} = \lambda^{2M-2} \qquad \textbf{Accuracy} \tag{25}$$

where

$$\lambda = k/h \tag{26}$$

is assumed constant, the above expansion reduces to

$$-\omega^2 + |\underline{\beta}|^2 + 2\sum_{M=2}^{M_i} \frac{(-1)^M k^{2M-2}}{(2M)!}\left(\omega^{2M} - |\underline{\beta}|^{2M}\right) = O(k^{2M_i}) \tag{27}$$

Furthermore, it is true that

$$\omega^{2M} - |\underline{\beta}|^{2M} = \left(\omega^2 - |\underline{\beta}|^2\right) P_M(\omega^2, |\underline{\beta}|^2) \tag{28}$$

for some multinomial $P_M(\omega^2, |\underline{\beta}|^2)$, and thus

$$\left(-\omega^2 + |\underline{\beta}|^2\right)\left(1 + O(k^2)\right) = O(k^{2M_i}) \tag{29}$$

or

$$-\omega^2 + |\underline{\beta}|^2 = O(k^{2M_i}) \tag{30}$$

and thus the scheme approximates the 2D wave equation to $2M_i$th order.

## Stability

In order to examine stability, consider again the case of a time harmonic grid function. The symbol corresponding to the scheme is then

$$\frac{-4}{k^2}\sin^2(\omega k/2) = \delta_{\mathcal{Q}} \tag{31}$$

which is satisfied for real frequencies $\omega$ when

$$\max_{\beta_x,\beta_y} \delta_{\mathcal{Q}} \le 0 \qquad \lambda \le \lambda_{\mathcal{Q}}\left(\underline{\alpha}\right) = \frac{2}{\min_{\beta_x,\beta_y}\left(h\sqrt{-\delta_{\mathcal{Q}}}\right)} \qquad \textbf{Stability} \tag{32}$$

These serve as stability conditions for the scheme; in particular, $\lambda_{\mathcal{Q}}\left(\underline{\alpha}\right)$ is the maximal Courant number for a given parameterized set of approximations $\mathcal{Q}$ with weights $\underline{\alpha}$.

## OPTIMIZATION

The constraints above provide a framework for the optimization of schemes over the parameters $\underline{\alpha}$, and $\lambda$, the Courant number, which is not independent of $\underline{\alpha}$. The constraints (13) and (17) are linear in $\underline{\alpha}$. The constraint (25), however, is dependent on $\lambda$, and the range of available $\lambda$ is dependent on $\underline{\alpha}$, from the stability conditions (32). Thus the space of parameters $\underline{\alpha}$ to be explored is not simple.

Before defining a cost function, it is worth noting a constraint which is peculiar to audio.

First, note that, from (32), if for a given choice of parameters $\underline{\alpha}$, $\lambda$ is chosen away from its maximal value of $\lambda_{\mathcal{Q}}\left(\underline{\alpha}\right)$, there will be a loss of bandwidth—the scheme will not be capable of producing frequencies above $\omega_{max} = \frac{2}{k}\sin^{-1}\left(\lambda/\lambda_{\mathcal{Q}}\left(\underline{\alpha}\right)\right)$. Thus it may make sense to choose, a priori,

$$\lambda = \lambda_{\mathcal{Q}}\left(\underline{\alpha}\right) = \frac{2}{\min_{\beta_x,\beta_y}\left(h\sqrt{-\delta_{\mathcal{Q}}}\right)} \qquad \textbf{Stability(Strong)} \qquad (33)$$

so that, for a given parameter set $\underline{\alpha}$, $\lambda$ is determined.

The choice of a cost function in optimization is a very delicate matter. First, define the normalized wavenumber variables $\underline{\hat{\beta}} = h\underline{\beta}$. The numerical phase velocity can then be defined as

$$v_{\phi}(\underline{\hat{\beta}}) = \frac{\omega}{|\underline{\beta}|} = \frac{2}{\lambda|\underline{\hat{\beta}}|}\sin^{-1}\left(\frac{\lambda}{2}\sqrt{-h^2\delta_{\mathcal{Q}}}\right) \qquad (34)$$

which is dependent only on functions of the variable $\underline{\hat{\beta}}$ and $\lambda$, but not $k$ or $h$ explicitly. A mean square error can then be defined as

$$E(\underline{\alpha}) = \int_0^{\pi}\int_0^{\pi} w\left(v_{\phi}-1\right)^2 d\hat{\beta}_x d\hat{\beta}_y \qquad (35)$$

where $w = w(\underline{\hat{\beta}})$ is a weighting function—a useful choice of such a weighting function is one which selects wavenumbers $\underline{\hat{\beta}}$ with $|\underline{\hat{\beta}}| \leq \hat{\beta}_0$, for some $\hat{\beta}_0 \leq \pi$.

## SIMULATIONS

It is useful to compare numerical phase velocity contour plots, as a function of $0 \leq \hat{\beta}_x, \hat{\beta}_y \leq \pi$ under both modified equation methods, specifying an order of accuracy, and also under general optimization. For comparison, in Figure 2, such plots are given for simple nine point schemes, where variations of 0.5 % in numerical phase velocity are indicated by contours. The fourth plot shown, with $a_{1,0} = 2/3$ and $a_{1,1} = 1/3$ is the nine point optimized scheme (isotropic to fourth order).

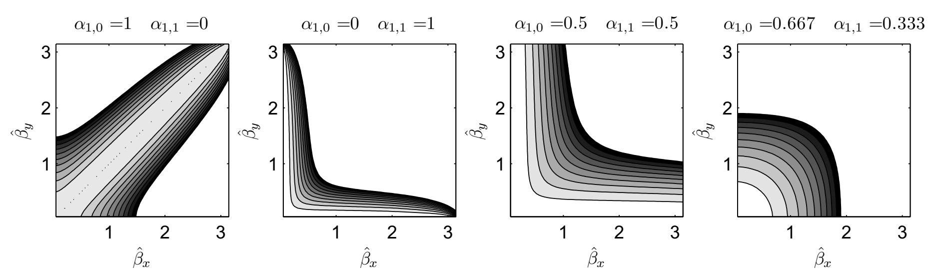


**FIGURE 2:** Phase velocity contour plots, with contours of 0.5%, for various members of the family of schemes with $\mathcal{Q} = \{(1,0),(1,1)\}$, with parameters $a_{1,0}$ and $a_{1,1}$ as indicated.

One choice one must make is that of the family $\mathcal{Q}$ of approximations; this choice, as it scales directly with computational cost, should be made a priori. As a first attempt at using modified equation methods, one can examine families $\mathcal{Q}$ for which $N_{\mathcal{Q}}$, the number of distinct approximations to the Laplacian is one more than the number of distinct constraints to be employed, giving a one parameter optimization over families of schemes of a given order of accuracy. $\lambda$ is assumed set according to the strong stability criterion (33). Modified equation schemes, of 4th, 6th and 8th order, for several choices of familes of grid points are shown in Figure 3. As all constraints refer to behaviour about spatial DC, as expected, there is an increasingly large flat region, encompassing, in the 8th order case, more than 2/3 of the wavenumber range of interest (with less that 0.5 % variation in wave speed.

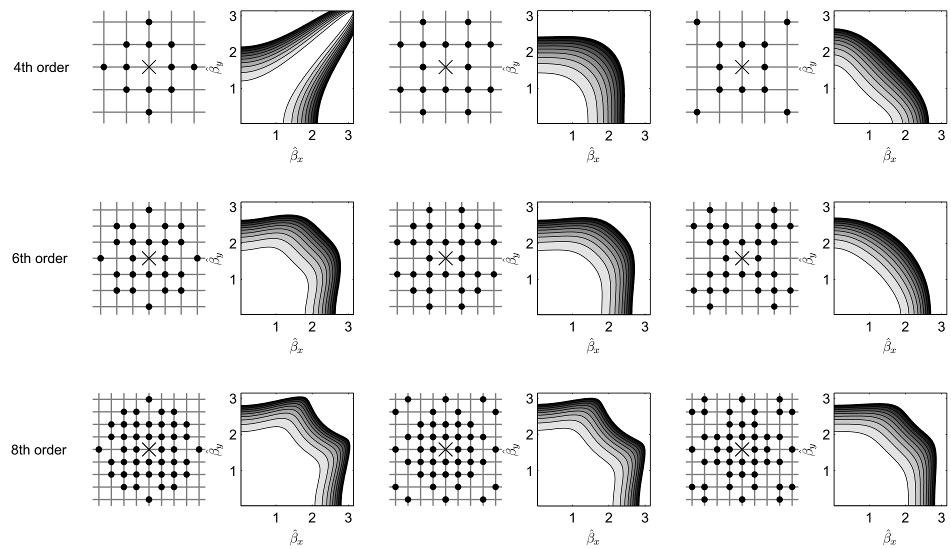


**FIGURE 3:** Numerical phase velocity contours for modified equation methods of 4th, 6th and 8th order, over a variety of choices of sets of grid points.

For comparison, one may attempt brute force optimization over these same families of grid points. Here, the mean square objective function (35) has been used

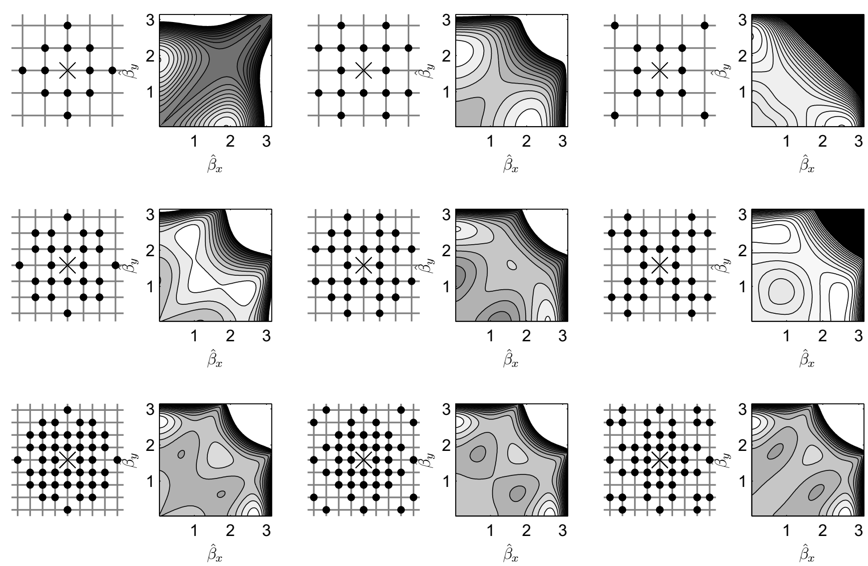


**FIGURE 4:** Numerical phase velocity contours for the choices of sets of grid points as illustrated in Figure 3, under optimization with the objective function given in (35), over a region of wavenumbers with $|\underline{\hat{\beta}}| \leq 0.95\pi$.

## CONCLUDING REMARKS

In this paper, parameterized families of wider stencil families for the 2D wave equation have been examined, and various constraints on the parameters, corresponding to consistency, isotropy, and accuracy have been introduced, allowing a means of developing optimization methods. The main benefit of such methods is that, despite the higher operation count, it is possible to obtain very low numerical dispersion over a very wide range of wavenumbers, allowing operation at a relatively low sample rate.

In terms of optimization, there are various issues of interest: one is in the specification of am appropriate objective function. Here, a simple mean square criterion has been proposed, but a maximum variation ($L^{\infty}$) measure is perhaps more appropriate. More generally, for applications in acoustics, the objective function should, ideally be framed in terms of psychoacoustic criteria. More problematic, however, is the problem itself—due to the interaction between the free scheme parameters and the Courant number through stability constraints (and, in the case of modified equation methods, accuracy constraints as well), it is not at all clear whether the optimization problem, regardless of the objective function chosen, possesses a unique minimum (or even a small number of such minima). Nevertheless, simple optimization methods, such as gradient descent do seem to converge to a global minimum in all cases examined here.

When boundary conditions are introduced, the termination of such schemes in such a way as to maintain numerical stability is a major consideration, and will be attacked in future work.

## ACKNOWLEDGMENTS

This work was supported by the European Research Council, under grant number StG-2011-279068-NESS.

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