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Should We Use the First- or Second-order Formulation with Spectral Elements for Seismic Modelling?

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SUMMARY

The second-order formulation of the wave equation is often used for spectral-element discretizations. For some applications, however, a first-order formulation may be desirable. It can, in theory, provide much better accuracy in terms of numerical dispersion if the consistent mass matrix is used and the degree of the polynomial basis functions is odd. However, we find in the 1-D case that the eigenvector errors for elements of degree higher than one are larger for the first-order than for the second-order formulation. These errors measure the unwanted cross talk between the different eigenmodes. Since they are absent for the lowest degree, that linear element may perform better in the first-order formulation if the consistent mass matrix is inverted. The latter may be avoided by using one or two defect-correction iterations. Numerical experiments on triangles confirm the superior accuracy of the first-order formulation. However, with a delta-function point source, a large amount of numerical noise is generated. Although this can be avoided by a smoother source representation, its higher cost and the increased susceptibility to numerical noise make the second-order formulation more attractive.

Introduction

Spectral methods for modelling seismic wave propagation are usually based on the second-order formulation of the wave equation, both for box-like elements on quadrilaterals and hexahedra (Komatitsch et al., 1999, e.g.) as well as for simplex-based elements on triangles (Mulder, 1996, 2013) or tetrahedra (Zhebel et al., 2014). For some applications, however, a first-order formulation may be desirable. Also, it can in theory provide much better accuracy in terms of numerical dispersion if the consistent mass matrix is used and the degree of the polynomial basis functions is odd (Ainsworth, 2014). Since inversion of this large sparse matrix is costly, mass lumping can be applied, but then the superior dispersion behaviour is lost. For that reason, Shamasundar et al. (2015) proposed the use of defect correction as an efficient alternative. In 1D, we found that one iteration with the consistent mass matrix, preconditioned by the mass-lumped mass matrix, reduced the numerical dispersion error. For the lowest-degree polynomial basis, the linear element, this enabled us to recover fourth-order super-convergence, two orders higher than with the second-order formulation of lowest degree. Lacking from that discussion was an analysis of the eigenvector error, describing the crosstalk between different element modes for degrees larger than one (Mulder, 1999). We will amend that here. Also lacking was the step to 2D and beyond. Below, we will present a simple Fourier error analysis for bilinear and triangular elements of lowest degree, to see if we can recover the fourth-order error behaviour observed in 1D on a highly regular mesh. Some numerical experiments are included.

Governing equations

We will consider the first-order formulation of the constant-density acoustic wave equation,

$$c^{-2}\partial_t p = \partial_x u + \partial_z v + f, \quad \partial_t u = \partial_x p, \quad \partial_t v = \partial_z p,$$

as well as the second-order formulation, $c^{-2}\partial_{tt} p = \partial_{xx} p + \partial_{zz} p + f'$. These are equivalent, but may differ after the spatial discretization. In the 1-D case, a finite-element discretization with spectral elements on Legendre-Gauss-Lobatto nodes produces first-derivative matrices, mass matrices, and, for the second-order formulation, a stiffness matrix. The first-order formulation involves three global mass matrices, which may or may not be lumped, the second-order formulation only one. In the 2-D case, we can discretize the equations with spectral elements on quadrilaterals, using the cartesian product of the 1-D basis functions, or on triangles, with tailor-made mass-lumped finite elements, for instance.

1-D eigenvalue and eigenvector errors

In 1D and on an equidistant mesh, the eigenvalues of the spatial operator describe the numerical dispersion. A discrete approximation of the spatial derivative, required in the first-order formulation, should provide an approximation $\mathrm{i}\kappa$ to the exact operator $\mathrm{i}\xi$, where $\xi = kh/M \in [-\pi, \pi]$ is a scaled version of the wavenumber k, h is the element size, and $M \geq 1$ the polynomial degree of the basis functions. The relative dispersion error is measured by $\kappa/\xi - 1$ and we can estimate its asymptotic behaviour of the form $\kappa/\xi - 1 \propto h^q$ for small h, where q is the exponent of the leading error term. In the second-order formulation, the eigenvalue κ^2 should approximate ξ^2 and we can define the relative dispersion error in the same way.

Apart from the eigenvalues of the spatial operator, we can determine its eigenvectors. One of those should correspond to the Fourier mode described by ξ or k. The others are 'spurious'. We can describe the cross talk between the mode by means of a matrix S, defined per element and of size $M \times M$. This matrix describes the amplitudes of the spurious modes relative to the unit size of the proper 'physical' mode — the Fourier mode we try to approximate. The entries of S also behave as h to some power for small h. Table 1 summarizes the exponents of the leading errors in the eigenvalues and eigenvectors of the 1D problem. The last column contains the suggested trends for interpolating degree $M > 1$, where it should be noted that exponents for the dispersion error in the second-order case were derived by Mulder (1999). Ainsworth (2014) gave a proof for the first-order case with a consistent mass matrix. The effect of the eigenvector errors dominates the results for degrees larger than one. Details are provided by Shamasundar and Mulder (2016). Numerical tests show that the overall error is dominated by the smaller of the two powers in Table 1.

The eigenvector errors reveal that the second-error formulation with mass lumping is to be preferred.

Table 1 *Exponents of the leading error in the dispersion curve and in the eigenvectors with LGL points and polynomials up to degree 5. The first of each pair corresponds to the relative error in the eigenvalue* $\mathrm{i}\kappa$ *for the first-order formulation or in the square root of the eigenvalue* κ^2 *for the second-order formulation. The second of each pair corresponds to the exponent of* ξ *in the leading error of the matrix S describing the eigenvector errors. This error is zero for* $M = 1$*. The last column shows expressions for the trend for* $M > 1$*, suggested by these results, where* $p(M) = M$ *if* M *is even and* $p(M) = M+1$ *if* M *is odd.*

order	mass matrix	$M=1$	2	3	4	5	trend $(M>1)$
1	consistent	4, –	4, 2	8, 4	8, 4	12, 6	$2p(M), p(M)$
	lumped	2, –	4, 2	6, 4	8, 4	10, 6	$2M, p(M)$
2	consistent	2, –	4, 4	6, 5	8, 6	10, 7	$2M, M+2$
	lumped	2, –	4, 4	6, 5	8, 6	10, 7	$2M, M+2$

An exception is the first-order formulation for the lowest degree, $M = 1$, with a consistent mass matrix. As already mentioned, the same fourth-order accuracy can be obtained with one iteration using the defect-correction principle. In the remainder, we will investigate this scheme more closely in two space dimensions.

2-D Fourier analysis

We can quickly analyse the performance in 2D by considering Fourier analysis on a periodic grid with square elements, both for bilinear elements and for linear elements on triangles. We start with bilinear elements on squares. Let T_x denote a shift operator in the x-direction, such that $T_x p_{k,l} = p_{k+1,l}$. Here, $p_{k,l}$ denotes the discrete pressure in the point (x_k, y_l) with $x_k = x_0 + kh_x$ and $y_l = y_0 + lh_y$ and grid spacings h_x and h_y. Its Fourier symbol is $\hat{T}_x = \exp(\mathrm{i}\xi_1)$ with $|\xi_1| \leq \pi$, where ξ_1 is related to the wavenumber k_x in the x-direction by $\xi_1 = k_x h_x$. Likewise, $T_y p_{k,l} = p_{k,l+1}$ with symbol $\hat{T}_y = \exp(\mathrm{i}\xi_2)$ with $|\xi_2| \leq \pi$. One row of the assembled mass matrix in a single node, relative to the others, is $\mathbf{M} = \frac{1}{36}\left[16 + 4(T_x^{-1} + T_x + T_y^{-1} + T_y) + T_x^{-1}T_y^{-1} + T_x T_y^{-1} + T_x^{-1}T_y + T_x T_y\right]$. Its symbol is $\hat{\mathbf{M}} = \frac{1}{36}(\hat{T}_x^{-1} + 4 + \hat{T}_x)(\hat{T}_y^{-1} + 4 + \hat{T}_y) = \frac{1}{9}(2 + \cos\xi_1)(2 + \cos\xi_2)$. One row of the derivative matrix in x is $\mathbf{D}^{(1)} = \frac{1}{12}(T_x - T_x^{-1})(T_y^{-1} + 4 + T_y)$, with symbol $\mathbf{D}^{(1)} = \frac{2}{3}\mathrm{i}(2 + \cos\xi_2)\sin\xi_1$. For $\mathbf{D}^{(2)}$, we can swap ξ_1 and ξ_2. Then,

$$\hat{\mathbf{M}}^{-1}\hat{\mathbf{D}}^{(1)} = \frac{3\mathrm{i}\sin\xi_1}{2 + \cos\xi_1} \simeq \mathrm{i}\xi_1(1 - \tfrac{1}{180}\xi_1^4),$$

showing that we have fourth-order accuracy with bilinear elements and a consistent mass matrix. With mass lumping, the result has only second-order accuracy: $\hat{\mathbf{M}}_{\mathrm{L}}^{-1}\hat{\mathbf{D}}^{(1)} = \frac{1}{3}\mathrm{i}(2 + \cos\xi_1)\sin\xi_1 \simeq \mathrm{i}\xi_1\left[1 - \frac{1}{6}(\xi_1^2 + \xi_2^2)\right]$. The expressions can be used to estimate the eigenvalues of $G = I - \mathbf{M}_{\mathrm{L}}^1\mathbf{M}$ by noting that

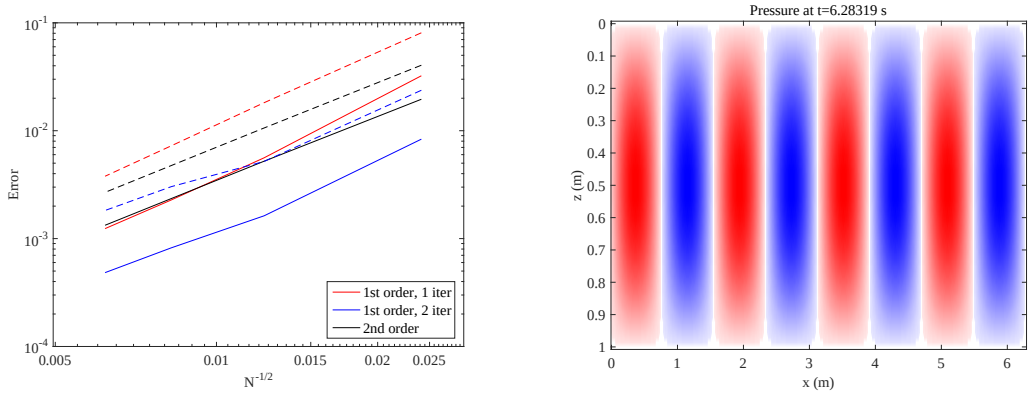
$$\hat{G} = 1 - \tfrac{1}{9}(2 + \cos\xi_1)(2 + \cos\xi_2) \in [0, \tfrac{8}{9}].$$

After one iteration with $\hat{G}$, the error becomes $-\frac{1}{180}\left(6\xi_1^4 + 10\xi_1^2\xi_2^2 + 5\xi_2^4\right)$, restoring the fourth-order accuracy.

We can repeat this analysis for linear elements on triangles and a regular mesh consisting of squares cut in half across the diagonal, from the left upper to the right lower corner. With unit spacing, the first triangle has vertices $(0,0)$, $(1,0)$, $(0,1)$ with basis functions $\{1-x-y, x, y\}$ and the second has $(1,1)$, $(1,0)$, $(0,1)$ with basis functions $\{-(1-x-y), 1-y, 1-x\}$. For the Fourier analysis, we select 8 triangles contained inside the 4 squares surrounding one node and assemble the matrices. Then, one row of the mass matrix is given by $\mathbf{M} = \frac{1}{12}(6 + T_x^{-1} + T_x + T_y^{-1} + T_y + T_x T_y^{-1} + T_x^{-1}T_y)$, with corresponding symbol $\hat{\mathbf{M}} = \frac{1}{6}(3 + \cos\xi_1 + \cos\xi_2 + \cos(\xi_1 - \xi_2))$. A row of the x-derivative matrix is $\mathbf{D}^{(1)} = \frac{1}{6}\left[2(T_x - T_x^{-1}) + T_y(1 - T_x^{-1}) + T_y^{-1}(1 - T_x)\right]$, with symbol $\hat{\mathbf{D}}^{(1)} = \frac{1}{3}\mathrm{i}(2\sin\xi_1 + \sin\xi_2 + \sin(\xi_1 - \xi_2))$. Now,

$$\hat{\mathbf{M}}^{-1}\hat{\mathbf{D}}^{(1)} \simeq \mathrm{i}\xi_1\left[1 - \tfrac{1}{360}\xi_1^2\left\{2\xi_1^2 - 5\xi_2(\xi_1 - \xi_2)\right\}\right],$$

revealing fourth-order behaviour of the error. The results for the derivative in the y-direction are the same after swapping T_x and T_y or ξ_1 and ξ_2. With mass lumping, the operator becomes $\hat{\mathbf{M}}_{\mathrm{L}}^{-1}\hat{\mathbf{D}}^{(1)} = \hat{\mathbf{D}}^{(1)} \simeq$



(a) (b)

Figure 1 *(a) Errors for the first-order formulation with one (red) or two (blue) defect-correction iterations, compared to the second-order formulation (black). The drawn lines correspond to the L2 errors, the dashed to the maximum errors. (b) Solution at final time.*

$i\xi_1\left[1-\frac{1}{6}(\xi_1^2+\xi_2^2-\xi_1\xi_2)\right]$, providing only second-order accuracy. These expressions also provide an estimate of the eigenvalue range of G: $\hat{G}=\frac{1}{6}\left[3-\cos\xi_1-\cos\xi_2-\cos(\xi_1-\xi_2)\right]\in[0,\frac{3}{4}]$. One iteration with $\hat{G}$ reduces the relative error to

$$-\frac{1}{360}\left(12\xi_1^4-25\xi_1^3\xi_2+35\xi_1^2\xi_2^2-20\xi_1\xi_2^3+10\xi_2^4\right),$$

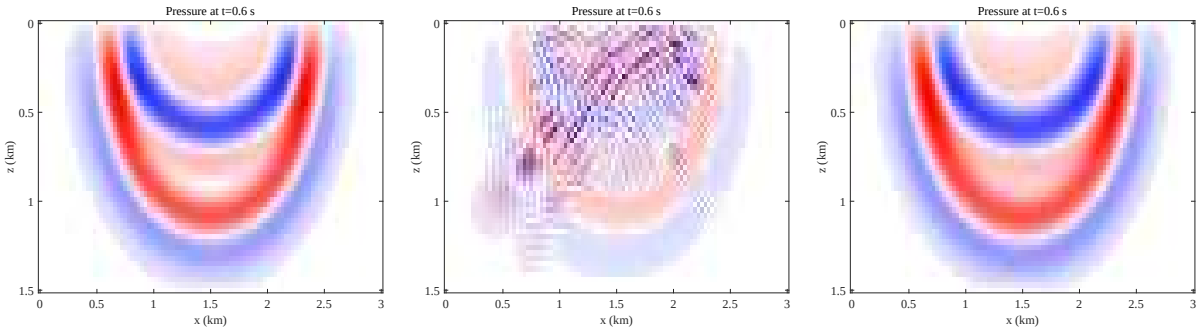
again restoring the fourth-order accuracy.

2-D numerical tests

A test problem is defined by $p(t,x,z)=\cos(\omega t)\sin(4x)\sin(\pi z)$ on the domain $[0,T]\times[0,2\pi]\times[0,1]$. We solve the constant-density acoustic wave equation with constant wave speed c_0 and $\omega=c_0\sqrt{4^2+\pi^2}$. The error is measured over all degrees of freedom at final time $T=2\pi/c_0$. Figure 1 shows errors for the first- and second-order formulation, using triangular finite elements of lowest degree. The coarsest mesh was based on a cartesian grid with 101×17 points. Each small rectangle was divided into two triangles. The finest mesh had 401×65 points or degrees of freedom. The first-order approach with two iterations of defect correction produces more accurate results in this case, although we appear to have difficulty to recover the fourth-order error behaviour estimated by the Fourier analysis. We should point out, however, that the error in the first-order formulation has a strong short-wavelength component, whereas the second-order formulation has a much smoother error in space.

As a second test problem, we took a rectangular domain with a point source and, for simplicity, constant density and sound speed, $c_0=1.5$ km/s, and zero boundary values for the pressure all around. The source was located in the centre at a depth of 250 m and had a Ricker wavelet with a 3-Hz peak frequency. Note that its time integral has to be used in the first-order formulation. The domain consists of 101×51 points, connected by triangles. Figure 2a shows the pressure wavefield at 0.6 s obtained with the second-order formulation, using a delta-function point source. This leads to a source representation by adjoint interpolation to nearby vertices using the basis functions. If we repeat this with the first-order formulation, we get the very noisy image of Figure 2b. Using a gaussian with a standard deviation of 50 m instead of a delta function produces the wavefield of Figure 2c. Apparently, the first-order formulation is sensitive to short-wavelength noise. In hindsight, this might have been anticipated, because the 1-D dispersion analysis produces curves that return back to zero at the shortest wavelength, meaning that this wavelength is not seen by the spatial operator. Once excited, it will not disappear. The gaussian source does not generate these modes, but will introduce some smearing of the wavelet, which in turn will increase the numerical error. Clever filter techniques may offer an alternative, but this has not been pursued.

We conclude that the first-order formulation of lowest order can be more accurate in some cases than the second-order formulation, but at a cost and with the risk of generating short-wavelength noise.



(a) (b) (c)

Figure 2 *Pressure field generated by a point source for (a) the second-order formulation with a delta-function point source, (b) the first-order formulation with a delta-function point source and no defect-correction iterations, and (c) with a gaussian source and two defect-correction iterations.*

Conclusion

We have shown that the eigenvalues of the spatial operator that describe the numerical dispersion alone do not provide sufficient clarity about the accuracy of numerical schemes. The error in the eigenvectors, which include the cross talk between different modes, should be taken into account as well. These errors are larger for the first-order than for the second-order formulation of the wave equation. Only for the lowest-degree scheme, with linear polynomials, the first-order formulation together with our iterative scheme is more accurate. Unfortunately, the scheme can be rather noisy, leading us to the conclusion that it is better to use the second-order formulation for any polynomial degree.

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