SANDIA REPORT
SAND200X-XXXX
Unlimited Release
Printed October 2016

Optimized Finite-Difference Coefficients for Acoustic Modeling

Leiph A. Preston

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Sandia National Laboratories

Issued by Sandia National Laboratories, operated for the United States Department of Energy by Sandia Corporation.

Printed in the United States of America. This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Telephone: (865) 576-8401
Facsimile: (865) 576-5728
E-Mail: reports@adonis.osti.gov
Online ordering: http://www.osti.gov/bridge

Available to the public from
U.S. Department of Commerce
National Technical Information Service
5285 Port Royal Rd.
Springfield, VA 22161

Telephone: (800) 553-6847
Facsimile: (703) 605-6900
E-Mail: orders@ntis.fedworld.gov
Online order: http://www.ntis.gov/help/ordermethods.asp?loc=7-4-0#online

SAND200X-XXXX
Unlimited Release
Printed October 2016

Optimized Finite-Difference Coefficients for Acoustic Modeling

Leiph A. Preston
Geophysics Department
Sandia National Laboratories
P.O. Box 5800
Albuquerque, New Mexico 87185-MS0750

Abstract

Although using standard Taylor series coefficients for finite-difference operators is optimal in the sense that in the limit of infinitesimal space and time discretization, the solution approaches the correct analytic solution to the acousto-dynamic system of differential equations, other finite-difference operators may provide optimal computational run time given certain error bounds or source bandwidth constraints. This report describes the results of investigation of alternative optimal finite-difference coefficients based on several optimization/accuracy scenarios and provides recommendations for minimizing run time while retaining error within given error bounds.

ACKNOWLEDGMENTS

This work was funded by the U.S. Department of Energy's Wind and Water Power Technologies Office.

CONTENTS

FIGURES

TABLES

NOMENCLATURE

FD	Finite-difference
PML	Perfectly Matched Layers
CPML	Convolutional perfectly matched layers
MPML	Multi-axial perfectly matched layers
O(2,4)	Second order accuracy in time; fourth order accuracy in space
CFL	Courant-Friedrichs-Lewy

1. INTRODUCTION

This paper briefly describes the implementation and testing of a variety of optimized second order in time and fourth order in space (O(2,4)) finite-difference coefficients for the acoustic propagation code Paracousti (Preston, 2016). Since coefficients can be optimized for a variety of criteria, seven different cases were studied to determine which one (or ones) produce the most accurate replication of a known analytical solution. Phase and group speed are two basic characteristics that can be easily calculated and optimized against for homogeneous media. The goal of this optimization is to find the coefficients for each test case that minimizes the required number of grid nodes per wavelength in order to match some maximum error bound. Since computational cost (run time) is proportional to the node spacing to the fourth power, even relatively small drops in the required number of grid nodes per wavelength can have large impacts on run time.

2. METHODS

2.1 Model Setup

All seven test cases use the same basic homogenous acoustic model. The acoustic sound speed (Vp) is set to 150 m/s throughout with 10 node thickness Convolutional Perfectly Matched Layer (CPML) boundaries on all sides. Model extents are 150 m by 200 m by 150 m. The source location in all cases is placed 40 m from the top (z) and left (x) sides of the model and in the middle of the model in the y-dimension. An explosive source with a 8 Hz gaussian waveform is utilized (the frequency refers to the spectral peak of the double differentiation of the gaussian pulse). Receivers are located on a line 60 m from the left side of the model and in the middle of the y-dimension, running top to bottom. Although all receivers were analyzed in these studies, only the receiver at 125 m from the top of the model are displayed in this report for examples. The time step and grid node spacing varied for each test case based on the computed grid nodes per wavelength required for the given optimized coefficients being tested.

2.2 Phase and Group Speed Equations

The equations for the numerical phase and group speed of the solution to the velocity-pressure system of equations on a standard staggered grid such as Paracousti are well known and given in Aldridge and Haney (2008). For completeness a summary is given here as well. For phase speed, assuming uniform grid spacing in each dimension for O(2,4) accuracy:

$$\frac{c_{phase}(s,\theta,\phi)}{c} = \frac{\sqrt{3}\left(|c_{inner}|+|c_{outer}|\right)}{\eta}\frac{1}{\pi s}\sin^{-1}\left[\frac{\eta}{\sqrt{3}\left(|c_{inner}|+|c_{outer}|\right)}Q(s,\theta,\phi)\right]$$

where

$$\begin{aligned} Q^2(s,\theta,\phi) = &\left[c_{inner}\sin(\pi s\sin\theta\cos\phi)+c_{outer}\sin(3\pi s\sin\theta\cos\phi)\right]^2 \\ &+\left[c_{inner}\sin(\pi s\sin\theta\sin\phi)+c_{outer}\sin(3\pi s\sin\theta\sin\phi)\right]^2 \\ &+\left[c_{inner}\sin(\pi s\cos\theta)+c_{outer}\sin(3\pi s\cos\theta)\right]^2 \end{aligned}$$

and c_{phase} is the numerical phase speed; c is the true phase/group speed; s is the sampling parameter ($s = h/\lambda$); h is the grid node spacing; λ is the wavelength of the propagating waveform; θ and ϕ are the angles of propagation relative to the z-axis and x-axis, respectively; c_{inner} and c_{outer} are the finite-difference coefficients; η is the ratio of the time step to the maximum time step allowed for stability (Courant-Friedrichs-Lewy (CFL) condition), given by:

$$\eta = \frac{ch_t}{h}\sqrt{3}\left(|c_{inner}|+|c_{outer}|\right)$$

where h_t is the time step.

The numerical group speed, c_{group}, is given by:

$$\frac{c_{group}}{c} = \frac{\delta}{\delta s}\left[\frac{c_{phase}}{c}s\right]$$

Given its complexity, the fully expressed formula will not be given here, but is fully derived in Aldridge and Haney (2008).

2.3 Procedure

All test cases, except the baseline case, use the same basic methodology. The baseline case is considered standard operating procedure; thus, maximum errors for the baseline case are used as bounding errors in all the other test cases. Maximum errors for the baseline case are 0.375% for phase speed, 1.2% for group speed, 2e-6 (unitless) weighted sum of square errors, and 3e-3 (unitless) sum of absolute errors.

Maximum (extremum) phase or group speed error refers to the maximum allowed percent deviation from the true phase or group speed curves. For a homogeneous medium the true phase and group speed curves are constant with respect to wavenumber (or frequency) and propagation direction and equal to the sound speed of the medium. However, in a numerical algorithm the numerical phase and group speeds do depend on wavenumber and propagation direction and tend to increasingly diverge from the ideal phase and group speeds as wavenumber increases, i.e., smaller wavelengths. These numerical phase and group speed curves also depend on the time step relative to the CFL time step limit and the finite-difference coefficients. The number of grid nodes per wavelength for any given combination of wave numbers, time step relative to CFL, and finite-difference coefficients is defined as the minimum wavenumber at which the numerical phase and/or group speed error exceeds the defined maximum error limits. Also, different directions of propagation are evaluated and the one that gives the strictest wavenumber is utilized.

The weighted sum of square (or absolute) errors also utilizes the phase and group speed curves, but it is the weighted sum of the square (or absolute) errors across all wave numbers that is the metric instead of maximum deviation. The weight function is a function of wavenumber and could, in principle be any arbitrary function. In all cases studied in this report, the weight function is the normalized spectra for a twice differentiated gaussian wavelet. This spectra is zero at zero frequency, peaks and then decays toward zero again at higher frequencies. The spectra is converted from frequency to wavenumber in order to form the weight function. This means that errors at very low wave numbers and also very high wave numbers will have minimal contribution to the total error, but instead the total error will be dominated by errors at wave numbers near the peak of the spectrum. In addition, group speed errors are weighted at approximately 1/3 of the phase speed errors at all wave numbers. Only the basic shape of the weight function is used. The wavenumber axis is stretched or compressed until the total error is approximately equal to the error limit. The maximum wavenumber having a spectral amplitude of 1% of the peak value of the spectrum is used to define the number of grid nodes per wavelength for the given time step relative to CFL and finite-difference coefficients. In addition, just as when using the error extremum, different propagation directions are utilized to find the strictest wavenumber for all directions.

3. TEST CASES

3.1 Baseline

The baseline case consists of using standard Taylor Series O(2,4) coefficients of 9/8 and -1/24 for the inner and outer coefficients, respectively. Also, the models are run at 99% of the CFL time step limit. We use 10 grid nodes per wavelength for the baseline case. This equates to a maximum phase speed error of 0.375% and group speed error of 1.2% (Figure 1). For this relatively small model with two compute domains it required 67 s run time. Results versus the analytic solution are shown in Figure 2. There is very good agreement between the solutions. For the following figures, the numerical phase and group speed curves are shown as a function of sampling parameter (s = wavelength per grid node) relative to the ideal (ideal = 1.0). CA = coordinate axis propagation; DB = body diagonal propagation. Also, comparisons of analytic to synthetic traces using a gaussian source time function are shown for each case.

3.2 Case 1: Optimized Taylor Series Time Step

This test case simply uses the same Taylor Series O(2,4) coefficients as in the baseline case, but a search is made to find the optimum time step relative to CFL condition that minimizes run time. Maximum error conditions of 0.375% for phase speed and 1.2% for group speed are used for the maximum error limits. The minimum computed run time occurs at 60% of the CFL limit with 6.16 grid nodes per minimum wavelength required to reach the same error tolerances as for the baseline case (Figure 3). This model required 15 s run time, a ~4.5x improvement over the baseline case, and it shows

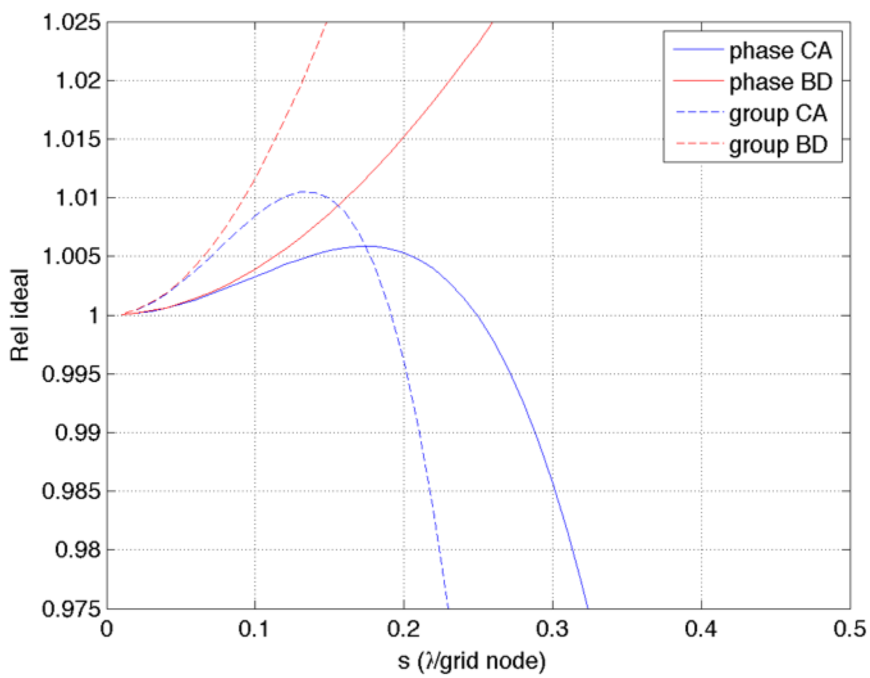

***Figure 1**: Baseline case phase and group speed curves*

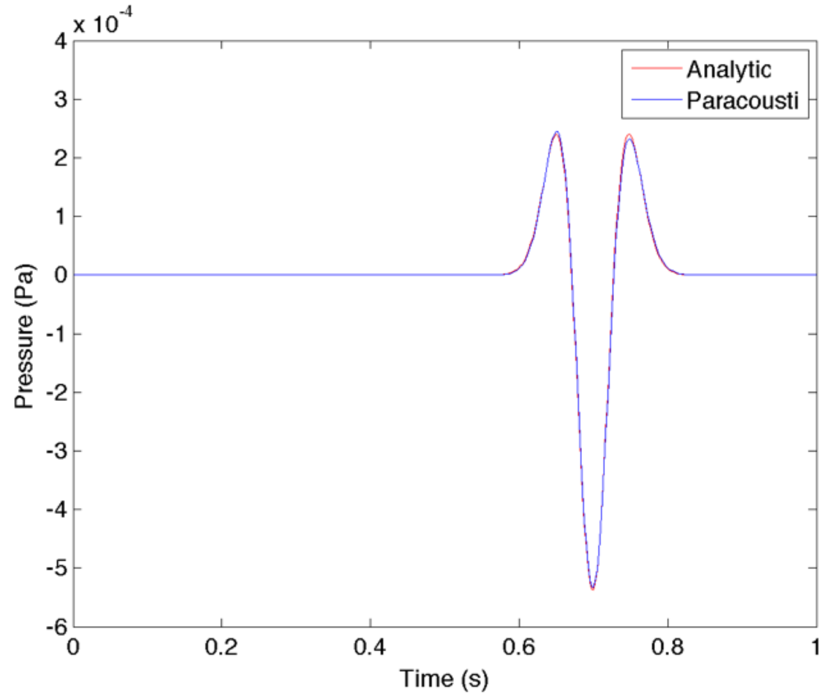

Figure 2: *Baseline case gaussian pulse*

excellent agreement with the analytic solution. This case actually had the closest agreement to the analytical solution of any of the cases run, including the baseline case (Figure 4).

3.3 Case 2: Optimized Coefficients for Phase Speed Only

This is the first case where the O(2,4) coefficients are allowed to vary in order to find the optimal run time. Only the phase speed curves were used in this case. The maximum phase speed error was set at 0.375%. The optimum run time was found to occur at 50% of the CFL limit for the inner and outer coefficients of 1.14337598613568 and -0.0490462530034956, respectively (Figure 5). These values give 4.46 grid nodes per minimum wavelength and required only 7 s to run, a nearly 10x improvement over baseline. However, the output traces are clearly not as good of a match to the analytic solution as baseline or Case 1 (Figure 6). Although the phases align reasonably well the amplitudes of the middle and last pulses are off by a few percent.

3.4 Case 3: Optimized Coefficients for Group Speed Only

This case is similar to Case 2 except that only the group speed curve is used to find the optimal run time. The maximum group speed error was set to 1.2%, the same as the group speed error of the baseline case. The optimum run time was found to occur at 60% of the CFL limit for the coefficients 1.14098247159559 and -0.0509925422379543 (inner and outer) (Figure 7). With these coefficients and time step a minimum of 5.07 grid nodes per minimum wavelength is required. This case took 8 s to run, amounting to over an eight-fold speedup compared to baseline. However, this is the poorest fit to

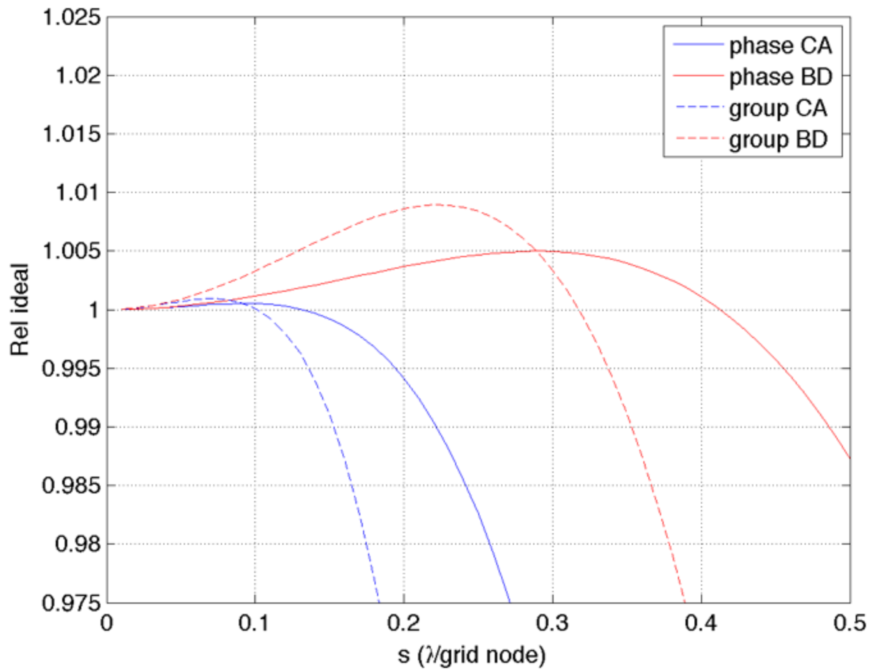

Figure 3: *Case 1 phase and group speed curves*

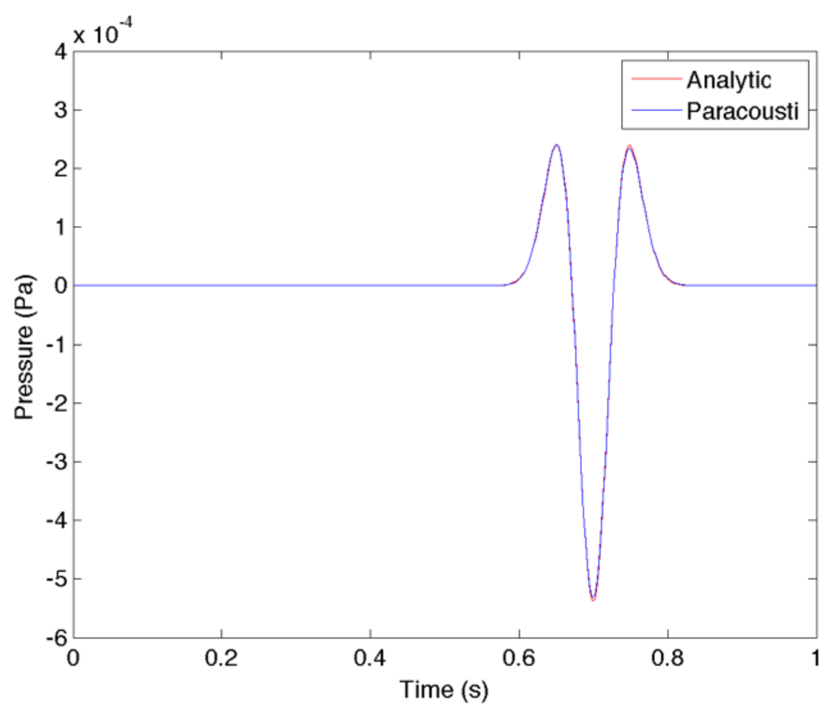

Figure 4: *Case 1 Gaussian Pulse*

the analytic solution of any of the cases tested. Clear phase misalignments are present with amplitude error as well (Figure 8).

3.5 Case 4: Optimized Coefficients for Phase and Group Speed

Due to the imperfections found in Cases 2 and 3, a combination of the phase and group speeds were used, setting maximum phase error to 0.375% and group speed error to 1.2%. In this case the optimum run time was found at 50% of the CFL limit for the inner an outer coefficients 1.14422873564654 and -0.0493171268197933 (Figure 9). These parameters give 5.22 grid nodes per minimum wavelength. This case required 11 s of run time, which is a factor of 6 improvement over the baseline. This case shows better fit to the analytic solution than either Case 2 or 3, but it still shows clear deviations in phase and amplitude compared to analytic (Figure 10).

3.6 Case 5: Optimized Coefficients for Weighted Square Errors

This case uses the sum of weighted square errors from both the phase and group speed curves, but with the group speed errors down-weighted by 1/3 at all wave numbers. As described above, the second time derivative of a gaussian pulse was used as the weight function in wavenumber space. The wavenumber of the peak of the gaussian was allowed to vary in order to find the weight function that gave a total error approximately equal to the limit of 2e-6. This is the same error as is found for the baseline case. The optimum run time was found to occur at 55% of the CFL limit for the inner and outer coefficients 1.12457173168659 and -0.041831528643767 (Figure 11). These parameters allow only 4.7 grid nodes per minimum wavelength. This case

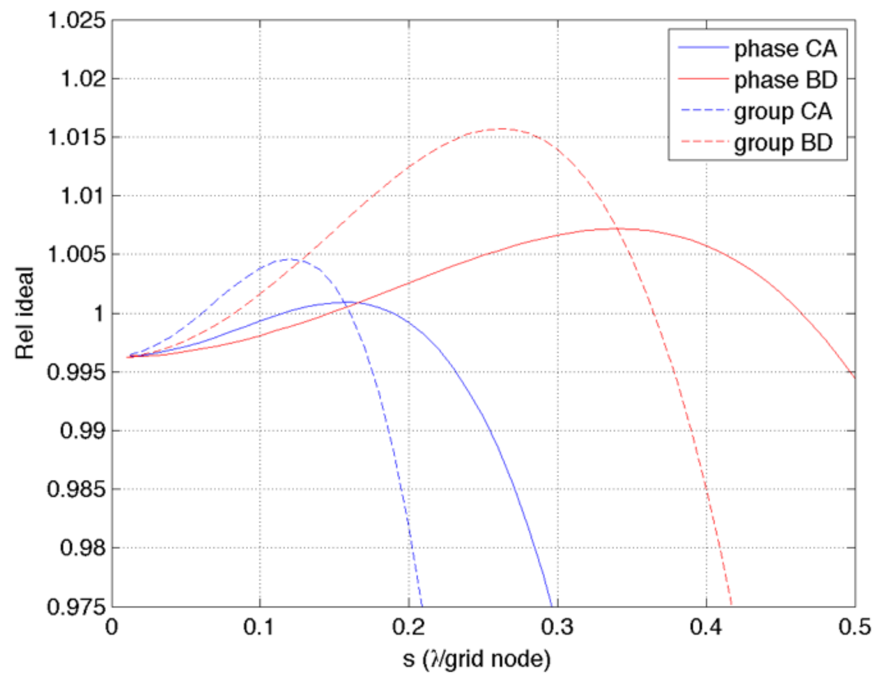

***Figure 5**: Case 2 phase and group speed curves*

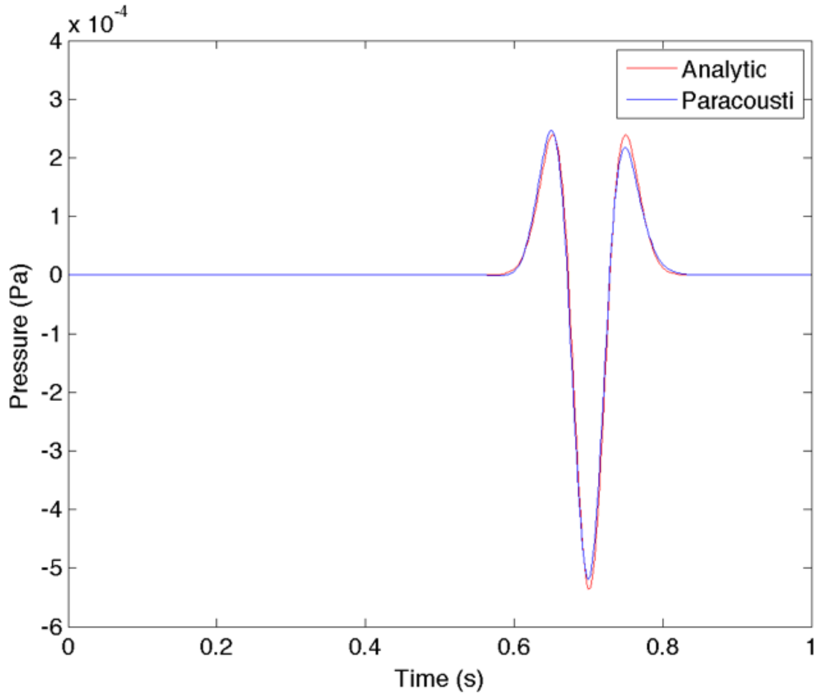

Figure 6: *Case 2 Gaussian Pulse*

required 7 s of run time, so, similar to Case 2, there is a nearly 10x run time improvement over the baseline case. In contrast to Case 2, the fit to the analytic solution is excellent in both phase and amplitude (Figure 12). This is the second best fit of all of the test cases, including the baseline, and is only minimally different than the Case 1 fit.

3.7 Case 6: Optimized Coefficients for Weighted Absolute Errors

This final case is similar to Case 5. The only difference is that the sum of the weighted absolute errors from both phase and group speed curves is utilized instead of square errors. An error limit of 3e-3 was used in this case, which is the same as that found for the baseline case. The optimum run time occurs at 45% of the CFL limit for the coefficients 1.1252025604248 and -0.0418246587117513 (Figure 13). With these parameters 5.05 grid nodes per minimum wavelength is required. This case required 10 s to run. It also shows a slightly worse fit to the analytic solution than baseline, Case 1 or Case 5, but it is still an excellent fit and a better fit than the other cases tested (Figure 14).

***Table 1**: Summary of cases, run times, and quality rank*

Case	Run time (s)	Quality Rank	Notes
Baseline	67	3	
1	15	1	Taylor, 60% CFL
2	7	6	Opt Phase Only
3	8	7	Opt Group Only
4	11	5	Opt Phase+Group
5	7	2	Opt Square Error
6	10	4	Opt Absolute Error

***Table 2**: Utilized finite-difference coefficients for each case*

Case	Inner Coefficient	Outer Coefficient	% CFL Limit
Baseline	1.125	-0.0416666666666667	99
1	1.125	-0.0416666666666667	60
2	1.14337598613568	-0.0490462530034956	50
3	1.14098247159559	-0.0509925422379543	60
4	1.14422873564654	-0.0493171268197933	50
5	1.12457173168659	-0.041831528643767	55
6	1.1252025604248	-0.0418246587117513	45

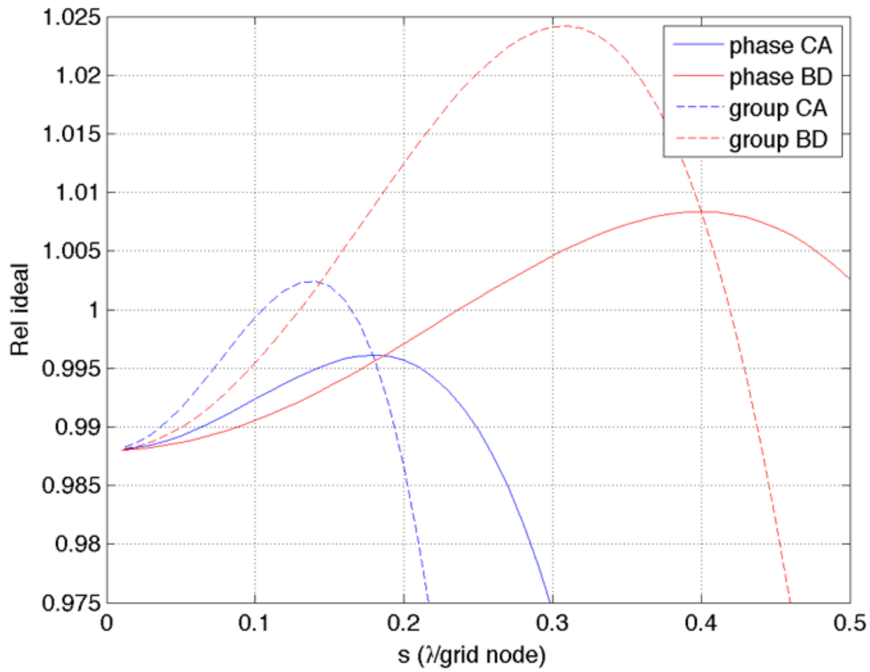

Figure 7: *Case 3 phase and group speed curves*

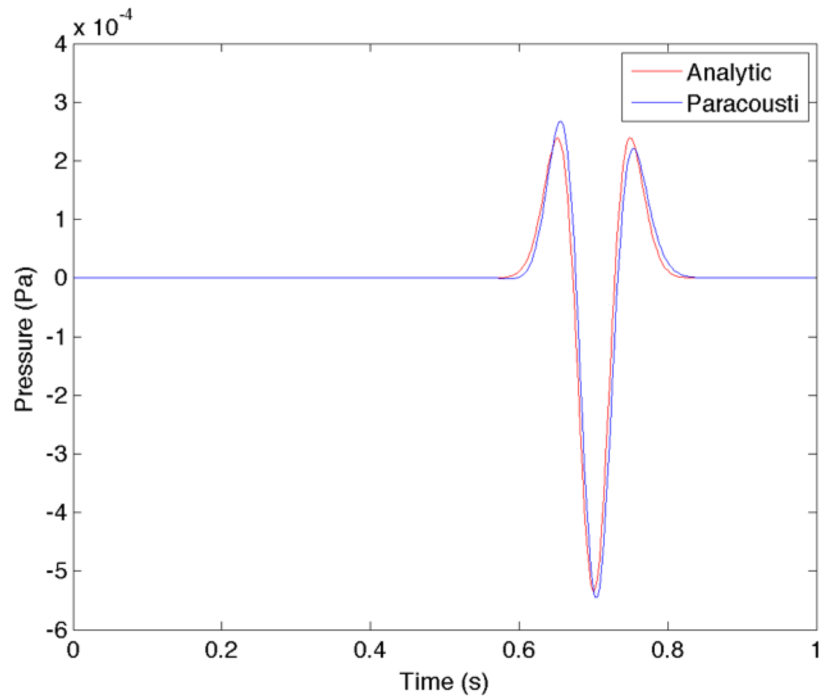

Figure 8*:* *Case 3 Gaussian Pulse*

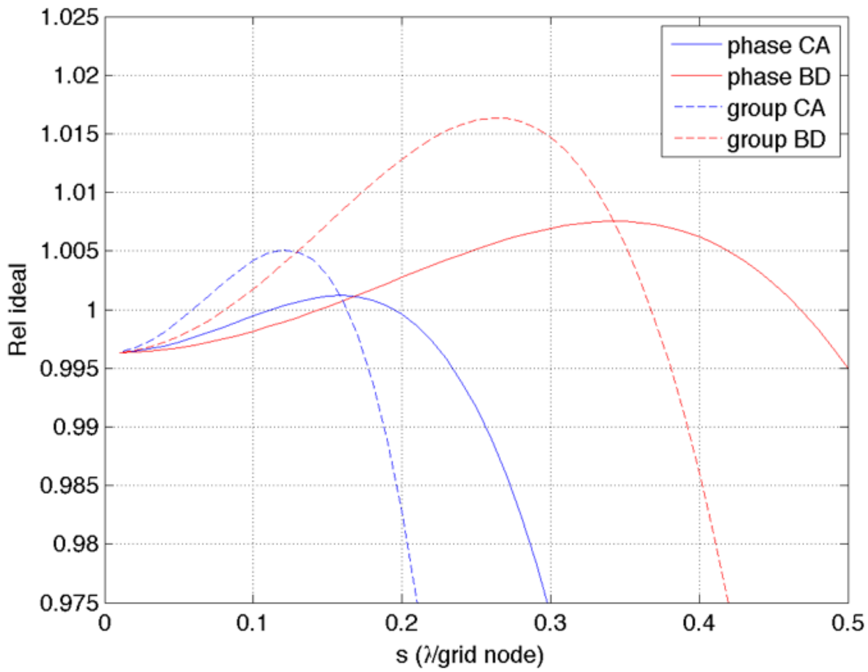

Figure 9: *Case 4 phase and group speed curves*

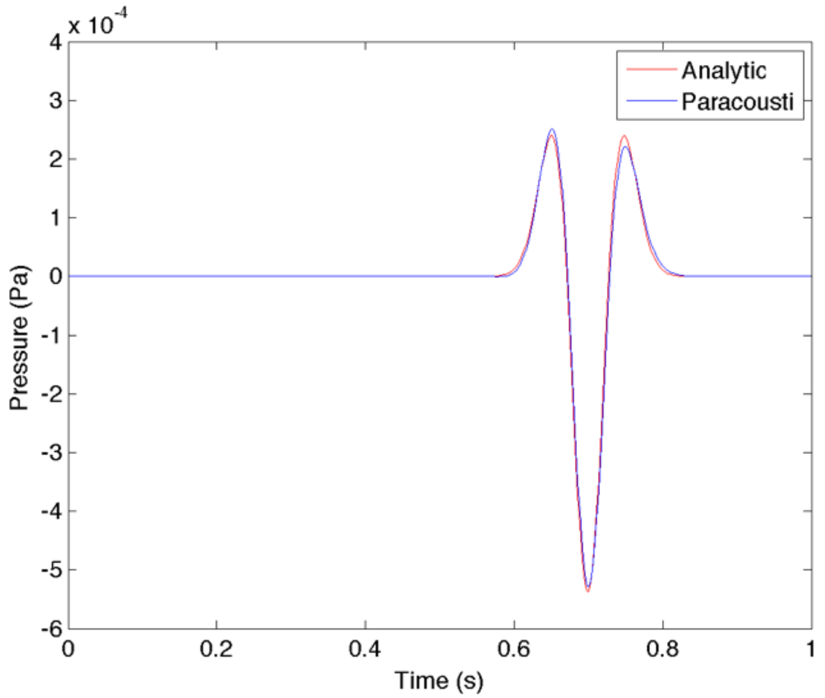

Figure 10*:* *Case 4 Gaussian Pulse*

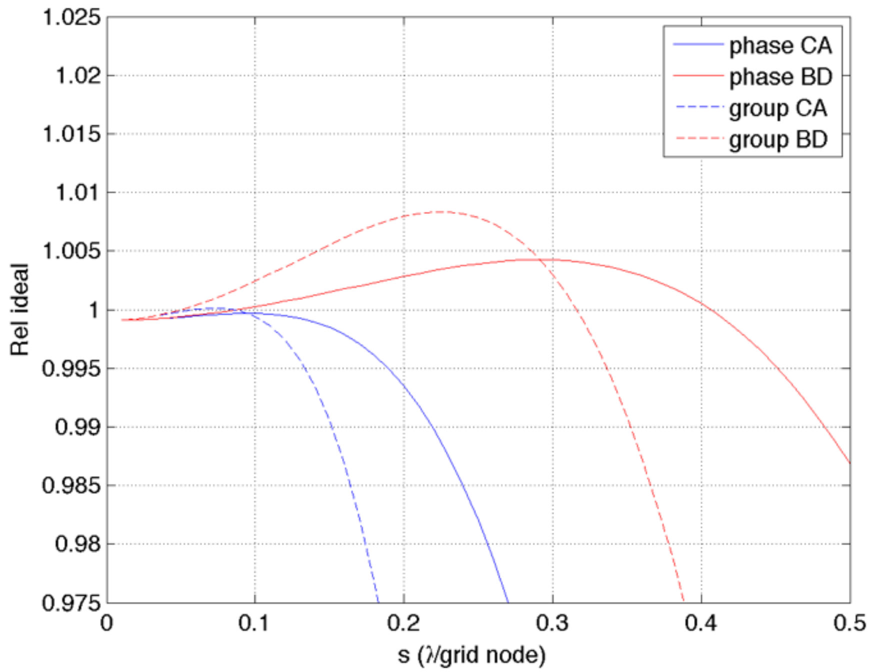

***Figure 11**: Case 5 phase and group speed curves*

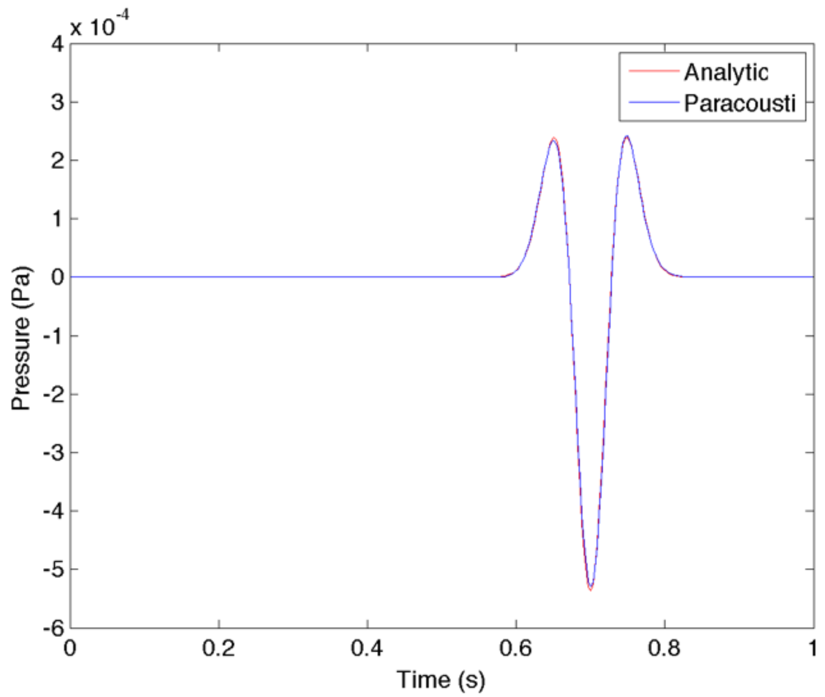

***Figure 12**: Case 5 Gaussian Pulse*

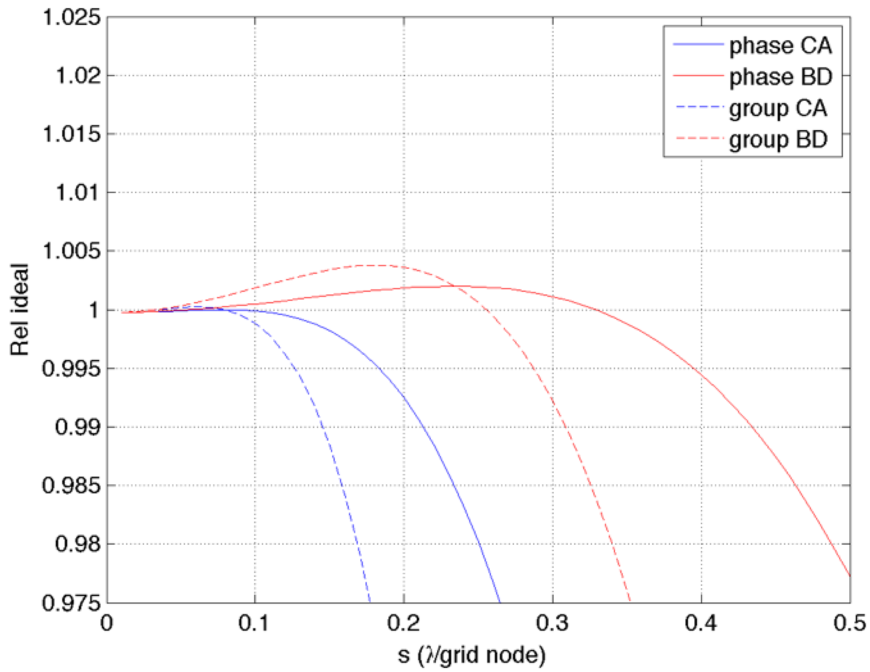

***Figure 13**: Case 6 phase and group speed curves*

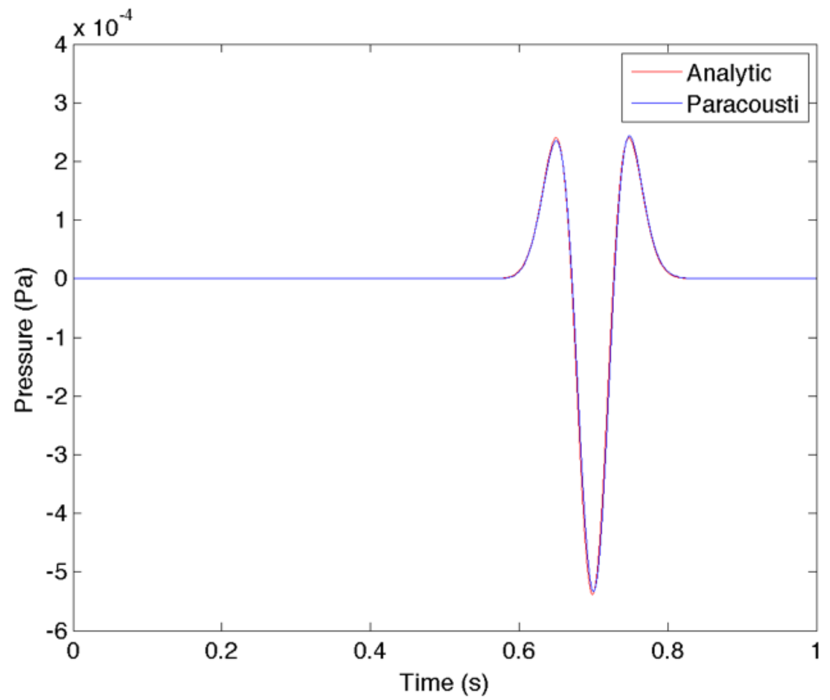

***Figure 14**: Case 6 Gaussian Pulse*

4. RESULTS AND DISCUSSION

4.1 Results Summary

As mentioned above and in Table 1, Case 1 has the highest quality fit to the analytic solution. However, the top four quality rankings all have excellent fits with only very small differences among them. Thus, any of the cases within the top 4 would be considered high quality and useable in synthetic calculations. These are the baseline case, Case 1, Case 5, and Case 6. Given that Case 5 runs over twice as fast as Case 1 and nearly 10 times as fast as the baseline case, this suggests that Case 5 would be the best choice. The one problem with Case 5 (and 6) is that they are not general. They are specific to only one family of source time functions that are self-similar in terms of wavenumber-scale invariance. However, it may be possible that some general source time functions could be sufficiently similar to the gaussian used here that these findings could be used in such a simulation and still have excellent results. As long as the frequencies where the general source is peaked have near-ideal phase and group speeds, the results still should remain valid. Of course, different weight functions, albeit self-similar, could also be utilized as a proxy for more general source time functions. However, if truly source agnostic results are needed, then Case 1 provides the best option of those studied.

4.2 Discussion

The standard Taylor Series coefficients and optimized weighted sum of errors provide the best fits to band-limited source time functions, whereas optimized coefficients for extremum errors are poorer. Below, I will discuss the qualities of each of these three classes of coefficients and its implication on the results.

The Taylor Series coefficients are based on fitting progressively higher order polynomials to a function in the neighborhood of a given point. As such, these are the only coefficients that will tend toward ideal at the low frequency (low wavenumber) limit. All other coefficients will tend to some non-ideal phase or group speed at the low frequency limit. Taylor coefficients do stray from ideal as frequency increases. Due to this fact, phase and group speed curves can exceed error limits at a lower frequency than may be possible for non-standard coefficients. However, since the Taylor coefficients stay in the vicinity of the ideal phase and group speeds over a broader bandwidth, we might expect that Taylor coefficients would be best for a general case where nothing is known of the source.

On the other hand, perhaps we can do better just by keeping phase and/or group speed curves within given error bounds out to higher frequencies than Taylor coefficients can permit. For example, maybe we can give up the requirement that in the low frequency limit that the solution goes to the correct phase and/or group speed if we know that the far field wavelet vanishes in the low frequency limit. By shifting the phase and/or group speed curves off ideal at low frequencies we can keep the curve within error bounds out to higher frequencies. Indeed, that is what the optimized coefficients based on maximal error bounds found. We can expand the frequency range, allowing a drop in run time by about a factor of 2 over Taylor coefficients. Unfortunately, there is still too much low frequency energy in the gaussian far field wavelet that the departure from ideal is too severe to provide an adequate fit. Of course, a different source wavelet with less low frequency content may show an improved fit, i.e., a more restrictive bandwidth of the source. Also, setting tighter error bounds would improve fit, but at the expense of longer run times.

An answer to the above issues is to use the total summed error over all frequencies and use information about the source to guide the optimization. This optimization allows the phase and group speeds to stray from ideal where the source has little energy and to match the ideal at the peak frequency of the far field source wavelet. So, the phase and group speed curves do not approach the ideal at the low frequency limit, but do stay closer to ideal throughout. The coefficients based on maximal error bounds tend to have their low frequency limit very near one (ideal). This maximizes the bandwidth over which the phase and/or group speed is within error bounds. However, instead of being nearly 0.375% in error, for example, in phase speed at the low frequency limit such as for the extremum error cases, the coefficients based on sum of errors is less than 0.1% in error at the same limit. Thus, low frequency energy in the source is more accurately propagated.

5. CONCLUSIONS

This report has described results of optimization studies for finite-difference coefficients in order to minimize run time within given error bounds under a variety of error bound measure scenarios. Case 1, standard Taylor Series coefficients with variable time step stability criteria, provides the best overall fit to analytic far field waveforms and should be used when nothing is known about the source. However, of nearly equal accuracy, but with half the run time, Case 5, which uses the weighted sum of square errors from both the phase and group speed, provides the best option if information about the source is known.

6. REFERENCES

1. Aldridge, D.F., and M.M. Haney, *Numerical dispersion for the conventional-standard-staggered-grid finite-difference elastic wave propagation algorithm*, SAND2008-4991, Sandia National Laboratories, Albuquerque, NM, July 2008.
2. Preston, L.A., *Paracousti user guide*, SAND2016-9291, Sandia National Laboratories, Albuquerque, NM, September 2016.

DISTRIBUTION

1	MS0750	Leiph Preston	6911
1	MS1124	Jesse Roberts	6122
1	MS0899	Technical Library	9536 (electronic copy)

Sandia National Laboratories