Getting it right without knowing the answer: quality control in a large seismic modeling project

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SUMMARY

Phase I of the SEAM Project will produce a variable-density acoustic synthetic survey over a 3D geological model simulating a deepwater subsalt exploration target. Due to the intended use of the data, the project places a premium on accuracy. Commercially produced Phase I synthetics will be spot-checked against benchmark simulations to assure quality. Thus the accuracy of the benchmark simulator required careful assessment. The authors designed and implemented the benchmark simulator used in this program, subjected it to verification tests, and assisted in the qualification phase of the Phase I project. The key lessons that we have learned so far from this assessment are that (1) the few verification tools available to us - a few analytic solutions and Richardson extrapolation - seem to be adequate, at least in a rough way, and (2) the standard approach to this type of simulation - finite difference methods on regular grids - requires surprisingly fine grid steps to produce small relative RMS errors for models of the type defined by this project.

INTRODUCTION

Large-scale simulation plays all sorts of roles in science and engineering, including design evaluation, ”what-if” contingency testing, and driving simulation-driven optimization. All such simulations consist in concatenating a large number of approximations of the underlying system of partial differential equations. Assessing the cumulative effect of these approximations is the *verification problem*: how close does the simulator come to solving the PDEs? Naturally, this question is most interesting when the simulator is really needed, that is, when the true solution is unknown!

Phase I of the SEAM Project (Fehler, 2009) provides an interesting opportunity for a verification study. The project aims to produce a synthetic survey over a state-of-the-art 3D geophysical model, emulating a subsalt exploration prospect in the deep water Gulf of Mexico. Numerical modeling provides the only means for simulating such data. The task is computationally large by contemporary standards. The model fills a 35 (E-W) $\times$ 40 (N-S) $\times$ 15 km cube with fine-scale simulated stratigraphy, rugose and massive salt bodies, and other features of exploration interest. Phase I requires roughly 65,000 shots (isotropic point radiator sources), for each of which 450,000 traces will be recorded, with intended fidelity to 25 Hz. The physics of Phase I wave propagation is variable density acoustics, and the model includes gridded compressional wave velocity and density fields.

Since the synthetic data will be produced by commercial entities whose methodology is opaque, SEAM required some independent mechanism for accuracy assurance. Project participants decided to assure data quality through use of a benchmark simulator, of known design and available for public inspection and use. The authors designed and tested this benchmark simulator, and assisted SEAM in designing a process for qualifying potential vendors, which included comparison of vendor and benchmark synthetics. Clearly the accuracy of the benchmark simulator is critical to the integrity of this quality assurance design.

We have learned two major lessons from our efforts to verify our benchmark simulator. First, the tools available to us, though distressingly limited, seem to be sufficient to give realistic assessments of simulator accuracy. Essentially only two methods are available: comparison with analytic solutions (in practice, this means homogeneous medium or perfectly reflecting half-space solutions); and error estimation by Richardson extrapolation (grid refinement). In the AIAA/ASME validation and verification taxonomy, these are known as “order” and “solution” verification respectively (AIAA, 1998).

Second, we found that regular-grid finite-difference simulation (Moczo et al., 2006), the standard modeling methodology for synthetic seismograms for the last several decades, suffers from severe accuracy limitations. Our benchmark simulator was of this type (a staggered grid (2,2k) scheme, described below). For reasons we will briefly review, all such codes are first-order convergent for models of the type used in SEAM Phase I, regardless of formal order of accuracy (Brown, 1984; Symes and Vdovina, 2008). Practically, this means that sample-by-sample accuracy is not particularly good, and obtaining small percentage RMS error is simply impossible with any reasonable grid refinement.

In the following paragraphs we will overview IWAVE, our benchmark simulator; explain the verification strategy employed in our study; review the accuracy limitations that afflict finite difference modeling with complex models; and discuss some of the results of our quality assurance tests for the qualification round of SEAM Phase I. We will end with a few remarks about possible directions for the evolution of seismic modeling technology. We regard the replacement of regular grid finite difference methods with dramatically more accurate methodology to be a very high priority, and see several possible avenues for improvement through the use of finite elements.

IWAVE: A BENCHMARK ACOUSTIC MODELING CODE

A code for the benchmark use described above must be

- based on well-understood principles;
- transparent (open source);
- verifiably accurate;
- fast enough for use in spot-checks of full-scale models;

Transparency and accuracy take precedence over speed.

IWAVE is a variable density acoustic simulator based on staggered grid finite difference approximation of linear acoustics, expressed in pressure-velocity form as

$$\frac{1}{\kappa(\mathbf{x})}\frac{\partial p(\mathbf{x},t)}{\partial t} = -\nabla\cdot\mathbf{v}(\mathbf{x},t)+f(t,\mathbf{x}), \quad (1)$$

$$\rho(\mathbf{x})\frac{\partial \mathbf{v}(\mathbf{x},t)}{\partial t} = -\nabla p(\mathbf{x},t). \quad (2)$$

Here the bulk modulus κ and material density ρ are functions of position $\mathbf{x}$. The right-hand side f in the first equation represents the source of acoustic energy as a constitutive law defect. For SEAM Phase I, $f(t,\mathbf{x}) = w(t)\delta(\mathbf{x})$, and the source wavelet $w(t)$ is chosen so that the presure field $p(\mathbf{x},t)$ has a desired far-field signature.

The staggered grid approximation replaces derivatives appearing in equations 1 with centered differences, defined on a regular rectangular grid (Virieux, 1984; Levander, 1988). IWAVE provides a variety of difference schemes of second order in time, and of user specified order between 2 and 14 in space. The current IWAVE application is built upon a *code framework* for finite difference simulation: it is structured to accommodate various intended extensions (Lax-Wendroff higher order time stepping, optimal stencil coefficients, various flavors of elasticity...). Package features include

- NPML (Hu et al., 2007) or pressure-release boundary conditions on any side of the domain boundary, at user option;
- 1D, 2D, or 3D simulation
- model input as gridded RSF/SEP file structure (Fomel, 2009), any sensible combination of velocity, bulk modulus, density, bouyancy, any axis order, any scale (units), native or XDR floats;
- data output as in SU format (SEGY without reel header) (Cohen and Stockwell, 2008)
- arbitrary source/receiver positions, sample rate via interpolation from computational grid
- calibrated to produce a specified wavelet at specified offset in free space;
- parallelization via domain decomposition and MPI, also at loop level via OpenMP, with simple user interface;
- parallelization over shots via subclustering;
- SU-style self-documentation.

A detailed description of the design, along with performance studies in various parallel environments, may be found in the second author's MA thesis (Terentyev, 2009).

SOLUTION VERIFICATION METHODS

Verification and validation have come to have standard meanings in the literature on computational simulation (AIAA, 1998). Crudely speaking, verification decides whether you're solving the equations right (computational accuracy), and validation whether you're solving the right equations (physical fidelity). SEAM pre-empts validation by asserting the adequacy of the linear acoustic model for the Phase I project. Verification is important for SEAM for at least two reasons. First, evaluating seismic modeling technology and stimulating its improvement are explicit project goals. Second, the simulation task is to be contracted to one or more vendors, who will use whatever methods they find convenient to produce synthetic traces. Thus SEAM must employ some form of quality control to ensure that the data are accurate enough to be useful for the purposes envisioned, and that the subsets produced by present and (possible) future vendors are compatible. [In February 2009 SEAM contracted with Tierra Geophysical for production of the Phase I data (Fehler, 2009).]

We used two methods of verification, called order and solution verification in the standard terminology. Order verification is simply the comparison with known (or manufactured) analytic solutions. The only analytic solutions available for this project, requiring only evaluation of elementary functions or interpolation (and not quadrature, for example, which must itself be verified) are the free space radiation solution and its modification by the method of images for a perfectly reflecting half space.

All other verification involves estimating the error between the numerical solution and an *a priori* unknown exact solution. The only effective technique known to us is *Richardson extrapolation*, also known as deferred approach to the limit and various other names (Kincaid and Cheney, 1996). It involves two assumptions, one theoretically verifiable in some cases, the other untestable in principle. Assume that computed data $D(\Delta t)$ differs from exact data $\bar{D}$ by

$$E(\Delta t) = C\Delta t^p + O(\Delta t^{p+1}). \quad (3)$$

Then, *assuming that the principal error* $C\Delta t^p$ *is dominant*,

$$E(\Delta t) \simeq \frac{D(2\Delta t) - D(\Delta t)}{2^p - 1}. \quad (4)$$

With little more work, one can estimate p from $D(\Delta t)$, $D(2\Delta t)$, and $D(4\Delta t)$. We emphasize that Richardson extrapolation (equation 4) is like most statistical estimation, in that it is *contingent* on an assumption which can only be made plausible, never actually verified.

LIMITED ACCURACY OF FINITE DIFFERENCE SIMULATION WITH COMPLEX MODELS

It has been known at least since the work of Brown (1984) that finite difference methods applied to wave problems with discontinuous coefficients (material parameters) are generically of first order accuracy, regardless of the formal order. The error splits into a familiar part governed by the truncation error, and a first-order part due to discontinuities in solution first derivatives at material interfaces. Use of higher order schemes controls the first part, which is responsible for grid dispersion, but does not affect the second part (Gustafsson and Wahlund, 2004). *Stairstep diffractions* are a widely known manifestation of the second category of error. We have analyzed this error component in detail in Symes and Vdovina (2008). Essentially, sampling the coefficients identifies the locations of interfaces only within the diameter of a grid cell, so the reflection arrival time may be in error by as much as the transit time of a cell. For some schemes, the second error component vanishes when material interfaces are aligned with grid planes (Brown, 1984). As we have shown (Symes and Vdovina, 2008), staggered grid schemes are denied even this pleasure: at least one of the grids carrying one of the physical fields is always misaligned. In fact, we have shown that the equation 3 is not even quite valid with $p = 1$; the constant C is not constant, but varies over a range depending on the exact relation between grid and discontinuities in κ or ρ. Still, as illustrated in (Symes and Vdovina, 2008), the Richardson estimation procedure (equation 4) still appears to give quite accurate results. It also shows that "first order" is effectively synonymous with "large": it is easy to construct simulations for which the conventional gridpoints-per-wavelength criteria are more than satisfied, but in which RMS errors of reflections are over 100%.

VERIFICATION AND COMPARISON OF SOLUTIONS

In the qualification stage of SEAM Phase I, the project received data from a number of potential vendors. As described by Fehler (2009), these data included traces from (1) homogeneous half space with pressure-free surface, (2) a dipping layer embedded in the half space, and (3) two shot positions to be simulated over a preliminary version of the SEAM model. Comparison of the submitted traces with analytic solutions (order verification) eliminated some of the submissions from further consideration.

An E-W slice through the SEAM velocity model at the position of qualification shot 1 appears as figure 1. The complexity of the model is evident in this cross-section.

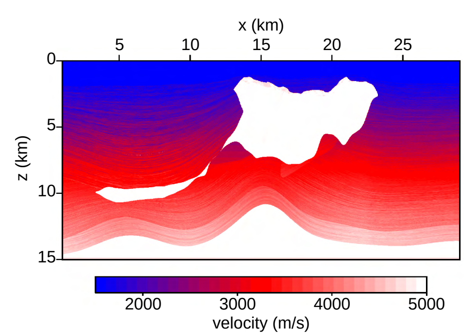


Figure 1: E-W section through SEAM velocity model through location of qualification shot 1 (E 15 km, N 17 km).

Figures 2 shows various time windows in several vendor-supplied traces at E 12 km, N 17 km for shot 1, along with the trace computed by IWAVE using a the (2,10) scheme and 10 m grid spacing. The traces shown are representative of the more accurate submitted results.

Unfortunately, the specification for the qualification data did not require that the amplitudes be calibrated, so the plots show traces independently normalized to unit maximum amplitude in each window. This mode of comparison understates the actual differences between the traces.

To gain a better idea of actual errors, we normalized each trace to have the same total energy over the first 8 s, and computed RMS relative differences with one of the vendor traces, in the first three windows displayed in Figure 2. Table 1 displays these errors, along with the estimated error in the IWAVE computed by Richardson extrapolation (equation 4 with $p = 1$) applied to 20 m and 10 m grid results.

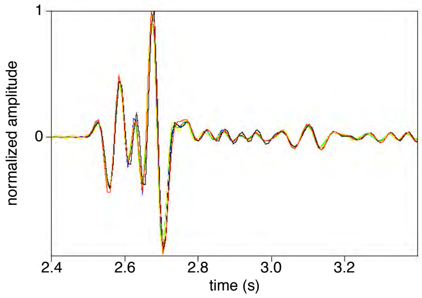
RMS Errors, 1 s windows			
window	2.4-3.4 s	5.5-6.5 s	7.0-8.0 s
blue	0.16	0.38	0.47
green	0.10	0.35	0.42
black	0.44	0.80	0.77
red (IWAVE)	0.30	0.55	0.63
Richardson	0.31	0.61	0.62

Table 1: Relative RMS errors in each window plotted in Figures 2(a), 2(b), and 2(c). Each row displays RMS error between one of the traces, identified by color in the plot, and the trace plotted in yellow, except for the last, which lists error estimates for the IWAVE trace derived by Richardson extrapolation.

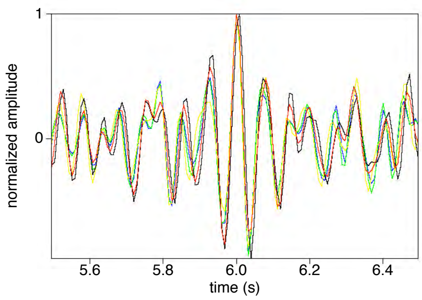
The most notable features of Table 1 are (1) the RMS errors beyond the water bottom event (Figure 2(a)) are quite large, on the order of 60%, and (2) Richardson extrapolation applied to IWAVE 20 m and 10 m output predicts that the IWAVE 10 m trace differs from the truth by about the same amount. From this we concluded that the Richardson "error bars" computed for the IWAVE solution did not suggest that any of the vendor results displayed in 2 are wrong. Similar exercises with other traces produced similar conclusions.

CONCLUSION

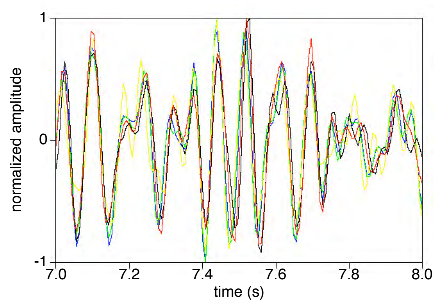
In one sense, the verification and quality assurance effort reported here was successful. The solution verification technique produced a usable error estimate for our benchmark simulator. Several vendors submitted plausible simulation results, which visually resemble those produced by our code. The variance of these results, taken together with ours, is approximately that suggested by Richardson extrapolation. This fact suggests both that the Richardson error estimate may be realistic, and that all of these results are as close to each other as the IWAVE result is to the truth. Therefore we cannot rule any of these submissions out as more inaccurate than the benchmark. The visual similarity of the traces also suggests that any of these



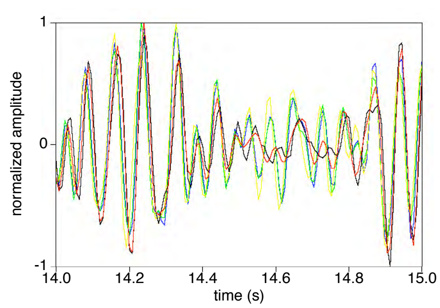
(a)



(b)



(c)



(d)

Figure 2: Traces at E 12 km, N 17 km for qualification shot 1 at E 15 km, N 17 km from four candidate vendors (blue, green, yellow, black) and IWAVE (red), in several time windows.

simulations should be equally useful for the intended imaging applications.

On the other hand, the estimated errors are distressingly large. It is also possible to attain a 60% error by scaling the true trace by 0.4, and that result would be unacceptable. In fact almost all of the differences between the traces compared in this study are due to small time shifts between events. We surmise that the origin of these time shifts is in the second category of finite difference error, discussed above. Various vendors used various finite difference schemes, but all are presumably contaminated with different versions of the second category error.

Reduction of the error to the proverbial engineering 5% would appear to require something other than regular grid finite difference methods. Several authors have proposed methods for reducing interface-related error over the years (for example Muir et al. (1992)). In at least one case, a reliable solution is known. We have recently shown rigorously that a multilinear (Q1) finite element scheme with mass lumping and numerical quadrature approximation of the stiffness matrix, applied to *constant density* acoustics, produces a pressure field free of second category error, even when discontinuities in bulk modulus do not align with the grid. The resulting method is computationally identical to a (2,2k) explicit difference scheme for the second order wave equation with specific spatial averaging of the bulk modulus (Terentyev and Symes, 2009). For more complex problems, the suppression of second category error requires more than mass lumping. The issue is well-known in the finite element wave propagation community - see for example the discussion in Cohen (2002). The commonplace fix in spectral element simulation of seismic response is use of unstructured meshes adapted to material discontinuities, see Komatitsch et al. (2005). Heterogeneity in the sedimentary column is too widespread and occurs at too many scales for this to be a practical remedy for simulation of reflection seismograms. Instead, we see a possible avenue in *immersed finite element* methods (Li and Ito, 2006) and their recent generalization by Owhadi and Zhang (2008). These methods transfer sub-grid information to stencil coefficients in regular, non-adapted grids.

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