GEOPHYSICAL RESEARCH LETTERS, VOL. 23, NO. 10, PAGES 1175-1178, MAY 15, 1996

Highly accurate P-SV complete synthetic seismograms using modified DSM operators

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Abstract. In previous papers [*Cummins et al.*, 1994ab] (hereafter referred to as DSMI and DSMII respectively), we presented accurate methods for computing complete synthetic seismograms for SH and P-SV respectively in a spherical earth model. The SH calculations used computationally efficient modified matrix operators, but the P-SV synthetics were computationally intensive. *Geller and Takeuchi* [1995] (hereafter referred to as GT95) presented a general theory for deriving modified operators and gave the explicit form of the modified operators for the P-SV case in cylindrical or cartesian coordinates. In this paper we extend GT95's results to derive modified operators for the P-SV case in spherical coordinates. The use of the modified operators reduces the CPU time by a factor of about 5 without a loss of accuracy. 10 CPU min on a SPARC-20 workstation with one CPU are required to compute a profile of synthetic seismograms from DC to 20 sec period.

Theory

To invert waveform data for 3-D earth structure, it is necessary to be able to compute synthetic seismograms and their partial derivatives accurately and efficiently. The Direct Solution Method (DSM) [*Geller et al.*, 1990; *Hara et al.*, 1991; *Geller and Ohminato*, 1994] is well-suited to such computations. The present paper presents results only for the laterally homogeneous case, but extension of our results to the 3-D case is straightforward [e.g., *Cummins et al.*, 1994c].

We begin by summarizing the results of DSMII for the P-SV case. The subscript k corresponds to the node and the subscripts $p = 1$ or 2 correspond to vertical and horizontal components respectively. ℓ is the angular order ℓ, m is the azimuthal order m, and $L = \sqrt{\ell(\ell+1)}$. Due to the degeneracy of the problem, the matrix elements depend only on ℓ and are independent of m. We denote the matrix elements by $T_{k'p',kp}$ and $H_{k'p',kp}$ for the solid part of the medium, and $T_{kk'}$ and $H_{kk'}$ for the fluid part of the medium.

Paper number 96GL00973
0094-8534/96/96GL-00973$05.00

The DSM equation of motion is:

$$(\omega^2\mathbf{T} - \mathbf{H} + \omega\mathbf{R})\mathbf{c} = -\mathbf{g}, \tag{1}$$

where $\mathbf{R}$ enforces continuity conditions at fluid-solid boundaries.

We choose linear splines as the radially dependent part of the trial functions. Their explicit form is

$$X_k(r) = \begin{cases} (r - r_{k-1})/(r_k - r_{k-1}) & r_{k-1} < r \le r_k \\ (r_{k+1} - r)/(r_{k+1} - r_k) & r_k \le r < r_{k+1} \\ 0 & \text{otherwise}, \end{cases} \tag{2}$$

where $r_0 < r_1 \cdots < r_N$.

We define the following intermediate integrals, which we call submatrices, for the solid part of the medium:

$$\begin{array}{ll} I^0_{k'k} = \int \rho r^2 X_{k'} X_k dr & I^1_{k'k} = \int \lambda X_{k'} X_k dr \\ I^2_{k'k} = \int \lambda r X_{k'} \dot{X}_k dr & I^3_{k'k} = \int \lambda r^2 \dot{X}_{k'} \dot{X}_k dr \\ I^4_{k'k} = \int \mu X_{k'} X_k dr & I^5_{k'k} = \int \mu r \dot{X}_{k'} X_k dr \\ I^6_{k'k} = \int \mu r^2 \dot{X}_{k'} \dot{X}_k dr & , \end{array} \tag{3}$$

where the dot denotes differentiation with respect to r. The integrals in (3) and (6), below, are non-zero only if $|k - k'| \le 1$. Using the above expressions, the matrix elements for the solid part of the medium are

$$\begin{array}{l} T_{k'1,k1} = T_{k'2,k2} = I^0_{k'k} \\ T_{k'1,k2} = T_{k'2,k1} = 0 \end{array} \tag{4}$$

and

$$\begin{array}{lcl} H_{k'1,k1} & = & 4I^1_{k'k} + 2(I^2_{k'k} + I^2_{kk'}) \\ & & +I^3_{k'k} + (L^2+4)I^4_{k'k} + 2I^6_{k'k} \\ H_{k'2,k2} & = & L^2 I^1_{k'k} + (2L^2-1)I^4_{k'k} \\ & & -(I^5_{k'k} + I^5_{kk'}) + I^6_{k'k} \\ H_{k'1,k2} & = & -L(2I^1_{k'k} + I^2_{kk'} + 3I^4_{k'k} - I^5_{kk'}) \\ H_{k'2,k1} & = & -L(2I^1_{k'k} + I^2_{k'k} + 3I^4_{k'k} - I^5_{k'k}). \end{array} \tag{5}$$

The rows and columns are ordered with p and p' changing most rapidly. This leads to both $\mathbf{H}$ and $\mathbf{T}$ being block tridiagonal, with each block having dimension 2×2 (Figure 1).

We define the following intermediate integrals for the fluid part of the medium:

$$I^{F0}_{k'k} = \int r^2 X_{k'} X_k / \lambda \, dr \quad I^{F1}_{k'k} = \int X_{k'} X_k / \rho \, dr$$
$$I^{F2}_{k'k} = \int r^2 \dot{X}_{k'} \dot{X}_k / \rho \, dr \quad . \tag{6}$$

The matrix elements for the fluid part of the medium are

$$T_{k'k} = I^{F0}_{k'k} \quad , \quad H_{k'k} = L^2 I^{F1}_{k'k} + I^{F2}_{k'k}, \tag{7}$$

where $\mathbf{T}$ and $\mathbf{H}$ are tridiagonal.

At the ICB (Inner Core Boundary) the indices are k^-_{ICB} for the node in the solid medium and k^+_{ICB} for the node in the fluid, while for the CMB (Core-Mantle Boundary) we have k^-_{CMB} for the fluid and k^+_{CMB} for the solid. The only non-zero elements of $\mathbf{R}$ are:

$$\begin{aligned} R_{k^-_{ICB}1, k^+_{ICB}} &= R_{k^+_{ICB}, k^-_{ICB}1} = r^2_{ICB} \\ R_{k^-_{CMB}1, k^+_{CMB}} &= R_{k^+_{CMB}, k^-_{CMB}1} = -r^2_{CMB}, \end{aligned} \tag{8}$$

where r_{ICB} and r_{CMB} are the radius at the ICB and CMB respectively.

Modified Operators

GT95 derived a general criterion for obtaining modified operators that greatly decrease the error of the solutions of eq. (1) without increasing the CPU time. GT95 presented modified operators for cartesian and cylindrical coordinates. We now extend their results to the P-SV case in spherical coordinates. $\mathbf{I}^3$ and $\mathbf{I}^6$ in eq. (3) and $\mathbf{I}^{F2}$ in eq. (6) are essentially 2nd derivative operators whose accuracy cannot be improved without using either a finer mesh or a higher order approximation. We use the results of GT95 to derive modified operators for the other integrals in eqs. (3) and (6) so that the error of the synthetic seismograms is minimized.

The various terms in eq. (5) fall into two categories. $\mathbf{I}^3$ and $\mathbf{I}^6$, $L\mathbf{I}^2$ and $L\mathbf{I}^5$, and $L^2\mathbf{I}^1$ and $L^2\mathbf{I}^4$ are all of comparable magnitude. On the other hand, terms such as the $\mathbf{I}^1$ or $\mathbf{I}^2$ terms in the first line of eq. (5) become comparatively negligible as ℓ increases; it is not necessary to replace such terms by a modified operator.

The elements denoted by open circles in Figure 1 are zero for the unmodified operators, but are non-zero for the modified operators. However, the CPU time required to solve eq. (1) does not increase, as the modified and unmodified operators both have the same bandwidth.

We do not modify $\mathbf{R}$. The modified operators $\mathbf{T}'$ and $\mathbf{H}'$ are defined as follows.

$$\begin{aligned} T'_{k'1,k1} &= T_{k'2,k2} = I^{0'}_{k'k} \\ T'_{k'1,k2} &= T_{k'2,k1} = 0 \end{aligned} \tag{9}$$

$$\begin{aligned} H'_{k'1,k1} &= 4I^{1'}_{k'k} + 2(I^2_{k'k} + I^2_{kk'}) \\ &\quad + I^3_{k'k} + (L^2+4)I^{4'}_{k'k} + 2I^6_{k'k} \\ H'_{k'2,k2} &= L^2 I^{1'}_{k'k} + (2L^2-1)I^{4'}_{k'k} \\ &\quad -(I^5_{k'k} + I^5_{kk'}) + I^6_{k'k} \\ H'_{k'1,k2} &= -L(2I^{1'}_{k'k} + I^{2'}_{kk'} + 3I^{4'}_{k'k} - I^{5'}_{kk'}) \\ H'_{k'2,k1} &= -L(2I^{1'}_{k'k} + I^{2'}_{k'k} + 3I^{4'}_{k'k} - I^{5'}_{k'k}) \end{aligned} \tag{10}$$

The submatrices, $I^0_{k'k}$-$I^6_{k'k}$ are defined above in eq. (3). $I^{0'}_{k'k}$, $I^{1'}_{k'k}$, $I^{2'}_{k'k}$, $I^{4'}_{k'k}$, and $I^{5'}_{k'k}$ are the newly defined modified submatrices.

$I^{0'}_{k'k}$, $I^{1'}_{k'k}$, and $I^{4'}_{k'k}$ correspond to operators that also appear in the SH problem. $I^{0'}_{k'k}$ is the same as $T^{mod}_{k'k}$ which is given in eq. (17) of DSMI. Note that W_k of eq. (17) corresponds to X_k in DSMII and this paper. $I^{4'}_{k'k}$ is the same as $H^{mod}_{(3)k'k}$ in eq. (17) of DSMI, and $I^{1'}_{k'k}$ is defined by replacing μ by λ in $I^{4'}_{k'k}$.

We consider a smoothly varying portion of the medium (with no discontinuities) and constant grid spacing, Δr. For the case of a discontinuity in elastic properties or Δr, we define the modified operators by "overlapping" (see Figure 1).

Following GT95, we derive the modified operators for $\mathbf{I}^2$ and $\mathbf{I}^5$ by dividing the quantities λr and μr into two parts. The major part is defined to vary stepwise, and the remaining part is the residual. We use the unmodified operators to calculate the matrix elements for the residual portions of λr and μr, and define modified operators for the step-wise varying parts. We consider a region in which Δr is constant. We define the intermediate variables, $(\lambda r)^{\text{step}}$ and $(\lambda r)^{\text{resid}}$ as follows.

$$(\lambda r)^{\text{step}} = \begin{cases} D_0 & r_0 \le r < r_0 + \Delta r/2 \\ D_k & r_k - \Delta r/2 \le r < r_k + \Delta r/2 \\ D_N & r_N - \Delta r/2 \le r \le r_N \end{cases} \tag{11}$$

$$(\lambda r)^{\text{resid}} = (\lambda r) - (\lambda r)^{\text{step}}, \tag{12}$$

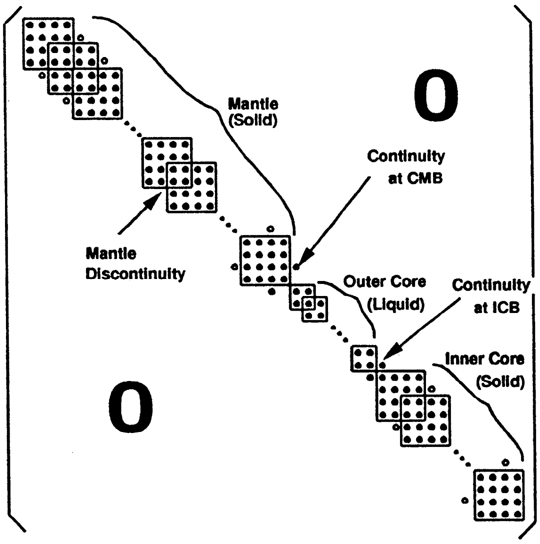

Figure 1. The structure of the original and modified operators. The solid circles are non-zero for both the original and the modified operators, and the open circles are non-zero for the modified operators only. However, the bandwidth of the unmodified and the modified operators are equal (7 for the solid regions and 3 for fluid regions), so the CPU time required to solve eq. (1) does not change.

where

$$D_k = \begin{cases} \dfrac{2}{\Delta r}\displaystyle\int_{r_k}^{r_k+\Delta r/2} \lambda r \, dz & (k=0) \\ \dfrac{1}{\Delta r}\displaystyle\int_{r_k-\Delta r/2}^{r_k+\Delta r/2} \lambda r \, dz & (1 \le k \le N-1) \\ \dfrac{2}{\Delta r}\displaystyle\int_{r_k-\Delta r/2}^{r_k} \lambda r \, dz & (k=N) \end{cases} . \quad (13)$$

$(\mu r)^{\mathrm{step}}$ and $(\mu r)^{\mathrm{resid}}$ are defined similarly.

Using $(\lambda r)^{\mathrm{step}}$, $(\lambda r)^{\mathrm{resid}}$, $(\mu r)^{\mathrm{step}}$ and $(\mu r)^{\mathrm{resid}}$, $I^{2'}_{k'k}$ and $I^{5'}_{k'k}$ are defined as follows:

$$I^{2'}_{k'k} = I^{2'\mathrm{step}}_{k'k} + I^{2'\mathrm{resid}}_{k'k} \quad (14)$$

$$I^{5'}_{k'k} = I^{5'\mathrm{step}}_{k'k} + I^{5'\mathrm{resid}}_{k'k} \quad (15)$$

$I^{2'\mathrm{resid}}_{k'k}$ is defined by replacing λr in the definition of $I^{2}_{k'k}$ in eq. (6) of DSMII by $(\lambda r)^{\mathrm{resid}}$. $I^{5'\mathrm{resid}}_{k'k}$ is defined by replacing μr in the definition of $I^{5}_{k'k}$ in eq. (6) of DSMII by $(\mu r)^{\mathrm{resid}}$. $I^{2'\mathrm{step}}_{k'k}$ and $I^{5'\mathrm{step}}_{k'k}$ are defined as follows:

$$\mathbf{I}^{2'}_{\mathrm{step}} = \frac{1}{12} \times \begin{pmatrix} -7D_0 & 8D_0 & -D_0 & & & \\ -5D_1 & -3D_1 & 9D_1 & -D_1 & & \\ & -5D_2 & -3D_2 & 9D_2 & -D_2 & \\ & & \ddots & \ddots & \ddots & \ddots \\ & & & -5D_{N-1} & -3D_{N-1} & 8D_{N-1} \\ & & & & -5D_N & 5D_N \end{pmatrix} \quad (16)$$

$$\mathbf{I}^{5'}_{\mathrm{step}} = \frac{1}{12} \times \begin{pmatrix} -5E_0 & -8E_1 & E_2 & & & \\ 5E_0 & 3E_1 & -9E_2 & E_3 & & \\ & 5E_1 & 3E_2 & -9E_3 & E_4 & \\ & & \ddots & \ddots & \ddots & \ddots \\ & & & 5E_{N-2} & 3E_{N-1} & -8E_N \\ & & & & 5E_{N-1} & 7E_N \end{pmatrix}, \quad (17)$$

where E_k is defined by replacing λ in eq. (13) by μ.

The modified operators for the liquid part of the medium are defined in basically the same way as the modified operators for the SH problem in DSMI. We therefore do not present explicit results in this paper.

Numerical Example

We present examples of P-SV computations for the isotropic part of the standard earth model, PREM [*Dziewonski and Anderson*, 1981]. Anelastic attenuation is also included in the computations.

We consider the period band 20-5000s (Figure 2). The source is a 600km depth, double-couple point source with a δ-function time history. $M_{r\theta} = M_{\theta r} = 1$, and all other components of the moment tensor are zero. The top synthetic in Figure 2 was computed using the modified operators with a very fine grid (3600 intervals), and we assume it is effectively exact. The second trace in Figure 2 shows a synthetic calculated using the modified operators with 1000 intervals, and the fourth trace shows a synthetic using the original operators with 1000 intervals. Both the second and fourth traces required 10 CPU minutes each, but the former is over 10 times more accurate. Only one trace is shown here, but a complete profile can be computed in essentially the same CPU time.

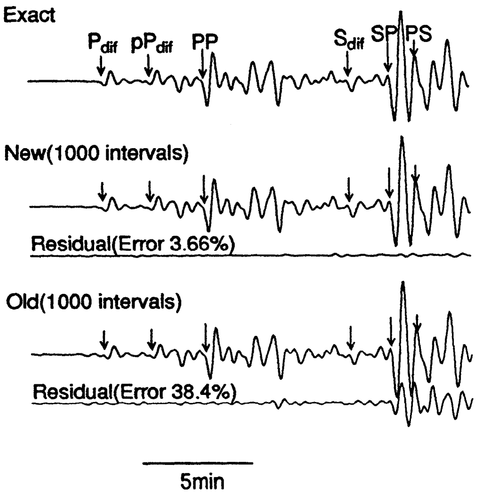

Figure 2. P-SV synthetic seismograms (vertical component) using the modified and the original operators. The source is a 600km depth point double-couple source, with $M_{r\theta} = M_{\theta r} = 1$ and all other components of the moment tensor zero. The top trace is an essentially exact solution computed using the modified operators with 3600 intervals. The second and the fourth traces show the numerical solutions using the modified and the original operators respectively, with 1000 intervals for each case. The third and fifth traces show the residuals for the second and fourth traces.

The third and the bottom traces show the residual between the numerical synthetics and exact synthetics for the modified and unmodified operators, respectively. The numerical error is larger for the S wave portions of the synthetic, as the vertical wavelength of S waves is shorter than that of P waves.

The last trace in Figure 2 shows that the synthetics computed using the unmodified operators are significantly out of phase with the exact waveforms, but a visual comparison of the "old" and "exact" synthetics might have led to the incorrect conclusion that the "old" synthetic was satisfactory. This underscores the importance of quantitative verification of the accuracy of synthetic seismograms, especially if they are to be used for waveform inversion.

Figures 3a and 3b show P-SV record sections computed using the modified operators. We used 18000 intervals (3400 intervals in the inner core, 6400 intervals in the outer core, and 8200 intervals in the mantle). The period band considered in this computation is 4-5000s;

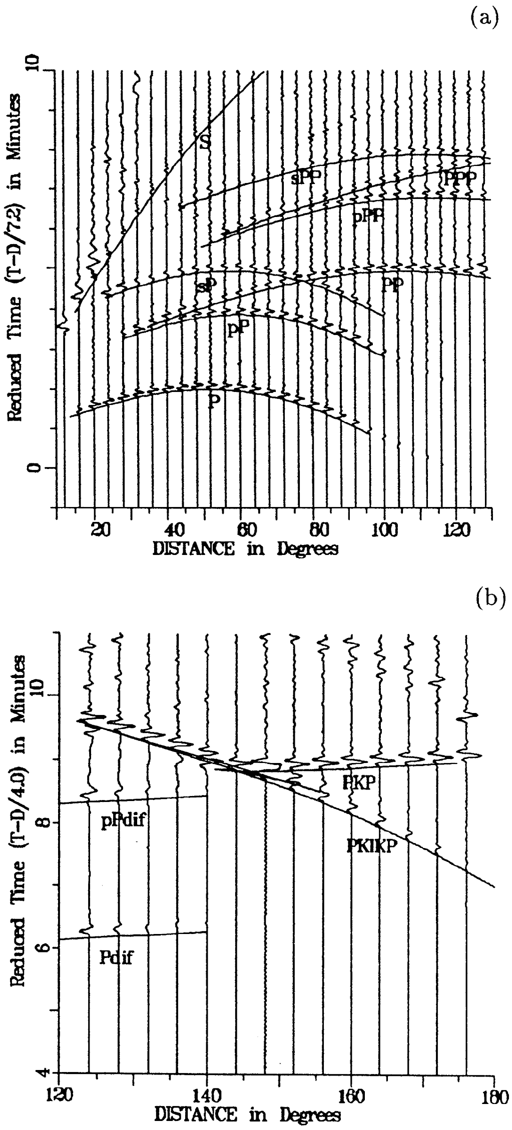

Figure 3. P-SV record section (vertical component) for the spherically symmetric model PREM. The source is the same as for Figure 2. (a) multiple reverberating P waves; (b) core phases.

a Butterworth low pass filter with a corner frequency of 0.15625Hz is applied to avoid a sharp cut-off at the Nyquist frequency.

Figures 3a and 3b show theoretical arrival times based on ray theory. The primary confirmation of accuracy is obtained by comparing the DSM and strong form solutions (details omitted due to space limitations). Note that as the arrival times are computed independently of the synthetics, the excellent agreement of the waveforms and travel times further confirms the accuracy of the synthetics. We plot only the first arrival of each phase in Figure 3a, so no triplications appear in the travel time curves. Figure 3b clearly shows the waveforms for PKP and PKIKP. About 60 hr on a SPARC-20 workstation using one processor was required to compute the synthetics in Figure 3.

There now seems to be a general consensus that tomographic studies of body wave travel times and surface wave phase velocities have reached a point of diminishing returns [e.g., *Nolet et al.*, 1994]. Synthetic seismograms computed using the modified operators presented in this paper should be highly useful for inverting for accurate and high resolution models of 3-D earth structure using long period body waves and surface waves.

Acknowledgments. We thank Jeff Park and an anonymous reviewer for helpful comments. We thank the Japan Society for the Promotion of Science for the support provided to N.T. for part of this work. This research was partially supported by a grant from the Japanese Ministry of Education, Science and Culture (No. 06640542) and by the ISM Cooperative Research Program (95-ISM-CRP-A-48).

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(received October 2, 1995; accepted January 18, 1996.)