

Efficient Modeling of Q for 3D Numerical Simulation of Wave Propagation

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Abstract The effects of Q are currently incorporated into numerical time-domain simulations of wave propagation by using a set of discrete relaxation functions. The behavior of these relaxation functions is controlled by the selection of the weight coefficients and relaxation times. In this article we present an approach to determine these parameters efficiently and accurately. In our approach we first determine two sets of weight coefficients and one set of relaxation times to model the smallest and largest target Q . We then derive an empirical formula to interpolate the weight coefficients for modeling an arbitrary Q that can be a function of frequency. A single set of relaxation times is used for any Q . We have considered two cases: (1) the complex viscoelastic material modulus is computed by directly summing of relaxation functions; (2) the modulus is implicitly represented as the harmonic average of the viscoelastic modulus given by individual relaxation functions. For large Q (>50), both approaches can be applied to coarse-grained system presented by Day and Bradley (2001). However, for lower Q , the second case works better.

Introduction

The intrinsic attenuation of seismic energy (often quantified by the quality factor Q) is an important consideration in the simulation of wave propagation. Although there is no difficulty incorporating an arbitrary Q , such as the frequency-independent Q of Kjartansson (1979) or the frequency-dependent Q of Müller (1983), into a frequency-domain simulation method, we are interested in including the Q effect in a time-domain simulation method, because such methods can simulate wave propagation in a complex medium. Currently Q is incorporated into time-domain numerical simulations by introducing additional memory variables (Day and Minster, 1984; Emmerich and Korn, 1987; Blanch *et al.*, 1995; Day and Bradley, 2001; Graves and Day, 2003).

In using memory variables, the attenuation and dispersion effects of Q are approximated by a set of relaxation functions. The linear combination of relaxation functions represents the modulus reduction from the unrelaxed modulus at time zero to the relaxed modulus at infinite time. The behavior of each relaxation function is simply controlled by a weight coefficient and a relaxation time. The more relaxation times that are used, the more accurate is the modeling of Q as a function of frequency. However, the number of different relaxation times is directly proportional to the number of memory variables; this proportionality directly affects the storage and computation time of the numerical methods. As an alternative to using many additional variables, Day (1998) and Day and Bradley (2001) presented a coarse-grained method that uses only one memory variable for each stress component of each node. This method dramatically

reduces storage requirements, but it introduces an artificial heterogeneity of the material modulus when the value of Q is very small. This undesired feature may degrade the accuracy of simulation of wave propagation (Graves and Day, 2003). Recently Graves and Day (2003) improved the performance of the coarse-grained method by using an element-specific unrelaxed modulus and an effective modulus, which is the harmonic average of the viscoelastic moduli over the coarse-grain unit. Moreover, in practical simulations of wave propagation the complex medium often contains more than tens of thousands of different Q values. Determining and storing the relaxation times and weight coefficients for these Q s is not a negligible task for most computers. To determine the weight coefficients efficiently, the low-loss approximation is often made for the modeling Q (e.g., Emmerich and Korn, 1987; Blanch *et al.* 1995; Day, 1998; Day and Bradley, 2001). If low Q values are included in a simulation, this approximation can be expected to result in notable error.

In this article, we extend and improve the procedure of Liu and Archuleta (1999) that determined the relaxation times and weight coefficients of the relaxation functions based on arithmetic averaging of the viscoelastic moduli. In the procedure that we develop later, we use one identical set of relaxation times for modeling different Q s; we optimize two sets of weight coefficients and the set of relaxation times to fit simultaneously the smallest and largest target Q (Q_{\min} and Q_{\max}). The weight coefficients for an arbitrary Q between Q_{\min} and Q_{\max} are interpolated in terms of an empirically derived relationship. We then apply this procedure to determine the relaxation times and weight coefficients when

the coarse-grained technique is implemented in the numerical simulation. In this case, the Q s are simulated using the harmonic average of the viscoelastic moduli over the coarse-grain unit. This procedure allows one to model both frequency-independent and frequency-dependent Q . In most cases we can simulate constant Q within 5% tolerance over three decades in frequency. The results we present here can be directly adapted to finite-difference algorithms with minimal storage requirements and minimal increase in computation.

Basic Formulas for Modeling Q

To incorporate the effects of Q into timestepped numerical simulations of wave propagation, a set of particular relaxation functions are chosen (e.g., Day and Minster, 1984; Emmerich and Korn, 1987) such that the complex, frequency-dependent, viscoelastic modulus $M(\omega)$ is approximated as,

$$M(\omega) = M_u \left(1 - \sum_{k=1}^N \frac{w_k}{1 + i\omega\tau_k} \right), \quad (1)$$

where M_u is the unrelaxed modulus; N is the number of relaxation times τ_k or weight coefficients w_k . In this case, as shown by Day and Minster (1984), the stress σ and strain ε has the relationship

$$\sigma(t) = M_u \left[\varepsilon(t) - \sum_{k=1}^N \zeta_k \right], \quad (2)$$

where ζ_k is the memory variable. The memory variables follow first-order differential equations (e.g., Day and Minster, 1984; Emmerich and Korn, 1987):

$$\tau_k \frac{d\zeta_k(t)}{dt} + \zeta_k(t) = w_k \varepsilon(t). \quad (3)$$

The difference solutions of these equations are of the form (Day, 1998)

$$\begin{aligned} \zeta_k(t + \Delta t/2) = & \exp(-\Delta t/\tau_k) \zeta_k(t - \Delta t/2) \\ & + w_k [1 - \exp(-\Delta t/\tau_k)] \varepsilon(t), \end{aligned} \quad (4)$$

where Δt is the timestep used in numerical calculation. We prefer to use $\exp(-\Delta t/\tau_k)$ in equation (4) rather than its first diagonal Padé approximant, $(1 - 0.5\Delta t/\tau_k)/(1 + 0.5\Delta t/\tau_k)$, because the latter can be negative when the relaxation time τ_k is very small.

Equation (2) provides a practical way to incorporate anelastic attenuation into the time-domain numerical simulation by introducing memory variables ζ_k . Equation (4) gives the approximate solutions of ζ_k , which are specified by τ_k and w_k . The accuracy of wave propagation with attenuation when using equation (2) depends on how well τ_k and

w_k are determined. In the following text and in the next section we present a procedure that uses an empirical interpolating relationship to calculate τ_k and w_k .

We use the definition of Q suggested by O'Connell and Budiansky (1978), and equation (1), to express the frequency-dependent Q as

$$Q(\omega) = \frac{\text{Re } M(\omega)}{\text{Im } M(\omega)} = \frac{1 - \sum_{k=1}^N \frac{w_k}{1 + (\omega\tau_k)^2}}{\sum_{k=1}^N \frac{w_k \omega \tau_k}{1 + (\omega\tau_k)^2}} \quad (5)$$

The simulated annealing algorithm of Liu *et al.* (1995) is used to find simultaneously N pairs of τ_k and w_k by minimizing the difference of a synthetic $Q(\omega)$ given by (5) and a target $Q(\omega)$ model. Here we extend and improve this technique such that we can determine all τ_k and w_k efficiently for different Q s. To do so, we first choose a minimum Q_{\min} and a maximum Q_{\max} . We assume that a single set of relaxation times τ_k can be used to simulate different Q s. Applying the simulated annealing algorithm (Liu *et al.*, 1995), we optimize two sets of w_k and one set of τ_k to fit simultaneously Q_{\min} and Q_{\max} . Having the weight coefficients $w_k^{\min Q}$ for Q_{\min} and $w_k^{\max Q}$ for Q_{\max} , the weight coefficients w_k^Q for any constant Q between Q_{\min} and Q_{\max} are interpolated by using an empirical formula that is obtained through numerical tests.

From a practical point of view, we set $Q_{\min} = 5$, $Q_{\max} = 5000$, $N = 8$, and the modeling frequency band 0.01–50 Hz. In this case, the weight coefficients w_k^Q for a given Q are calculated using the interpolation formula

$$w_k^Q = \chi(\chi\alpha_k + \beta_k), \quad (6a)$$

where the values of α_k and β_k are listed in Table 1. They are linear combinations of the weight coefficients $w_k^{\min Q}$ and $w_k^{\max Q}$. Although directly using $w_k^{\min Q}$ and $w_k^{\max Q}$ to interpolate w_k^Q looks more straightforward, equation (6a) is more efficient for computation. The factor χ depends only on Q and is estimated by

$$\chi = \frac{3.071 + 1.433Q^{-1.158} \ln(Q/5)}{1 + 0.415Q}, \quad 5 \leq Q \leq 5000. \quad (6b)$$

This formula was found by first deriving an analytical expression under many simplifying assumptions and then modifying the analytical expression based on the fit between the synthetic Q and the target Q . To verify the accuracy of the interpolation, we compute a series of synthetic Q s using equation (5). The frequency band is 0.01–50 Hz. These calculations use one set of relaxation times listed in Table 1. The weight coefficients are obtained from equation (6). In Figure 1 we plot the synthetic Q s and various target values of Q . Every synthetic Q (from 5 to 5000) fits the target value very well, although the fit is a little worse for large Q because

Table 1
Coefficients for Modeling Q , Equations (5) and (6)

k	τ_k	α_k	β_k
1	1.72333×10^{-3}	1.66958×10^{-2}	8.98758×10^{-2}
2	1.80701×10^{-3}	3.81644×10^{-2}	6.84635×10^{-2}
3	5.38887×10^{-3}	9.84666×10^{-3}	9.67052×10^{-2}
4	1.99322×10^{-2}	-1.36803×10^{-2}	1.20172×10^{-1}
5	8.49833×10^{-2}	-2.85125×10^{-2}	1.30728×10^{-1}
6	4.09335×10^{-1}	-5.37309×10^{-2}	1.38746×10^{-1}
7	2.05951	-6.65035×10^{-2}	1.40705×10^{-1}
8	13.2629	-1.33696×10^{-1}	2.14647×10^{-1}

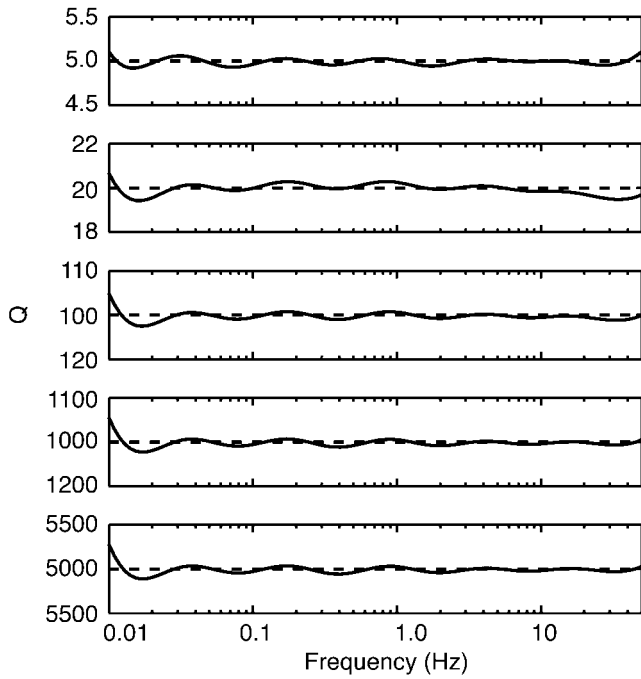


Figure 1. The fit between model Q (solid line) and the target $Q(\omega)$ (dashed line). Model Q is calculated using equation (5). The relaxation times $\bar{\tau}_k$ or weight coefficients w_k are obtained from Table 1 by use of equation (6).

we have given more weight to fitting the minimum Q . The misfits are less than 4% from 0.02 to 50 Hz. The largest misfits are within 8% tolerance at about 0.01Hz for very large Q .

Besides the calculation of relaxation times and weight coefficients, the other consideration in modeling Q is the determination of the unrelaxed modulus M_u (equation 1 or 2). A material velocity c used in numerical simulation is the phase velocity normally observed at specified reference frequency ω_r . The corresponding material modulus M_0 is represented as

$$M_0 = c^2\rho, \tag{7}$$

where ρ is the density. M_u is the modulus at infinite frequency, however, and it corresponds the initial value of the relaxation function and should be greater than the M_0 given by equation (7). Following the work of Day and Bradley (2001), we determine the M_u in a way that the modulus from equation (1) at frequency ω_r is equal to M_0 . With this consideration, we combine equations (1) and (7) to give a expression for the unrelaxed modulus:

$$M_u = c^2\rho \left/ \left| 1 - \sum_{k=1}^N \frac{w_k}{1 + i\omega_r\tau_k} \right| \right. \tag{8}$$

Where there is no information that gives the frequency at which the velocity model is known, the value of 2π (1 Hz) is not a bad choice for ω_r .

Kjartansson (1979) presented a model to simulate frequency-independent Q . The modulus of this model has the form

$$M(\omega) = M_0(i\omega/\omega_r)^{2\arctan Q^{-1}/\pi} \tag{9}$$

where ω_r is the reference (angular) frequency. Although this model is hard to implement in time-domain numerical simulations, it exactly represents a constant Q model. We calculate the modulus at different frequencies from this model and the modulus from equation (1) for a constant Q of 10. Comparisons of the two-computed moduli $M(\omega)$ are shown in Figure 2. The real and imaginary components of both moduli are almost identical. These features confirm that our interpolating procedure correctly models constant Q .

Although Day and Bernard (1984) derived equation (1) for general Q functions, it has only been applied to model constant Q in the time-domain computations (e.g., Emmerich and Korn, 1987; Blanch *et al.*, 1995; Day and Bradley, 2001; Graves and Day, 2003). Through numerical tests, we find that if we properly optimize both the weight coefficients and the relaxation times, we can correctly model frequency-dependent Q and frequency-independent Q . Figure 3 shows an example of modeling frequency-dependent $Q(\omega)$. The solid lines represent simulations and the dashed lines are given by

$$Q(\omega) = \begin{cases} Q_0, & \omega \leq \omega_c \\ Q_0\left(\frac{\omega}{2\pi}\right)^p, & \omega \geq \omega_c \end{cases}, \tag{10}$$

where, $Q_0 = 20$; $\omega_c = 2\pi$; the power p is 0.5 and -0.5 in Figures 3a and b, respectively. The weight coefficients for different frequency-dependent Qs can also be interpolated using a formula similar to equation (6), as long as these Qs are described with a common ω_c and power p .

Directly applying equation (2) to a time-domain numerical method, such as the finite-difference (FD) method, one finds that N memory variables are needed for each stress component in each cell. In practice N should be four or

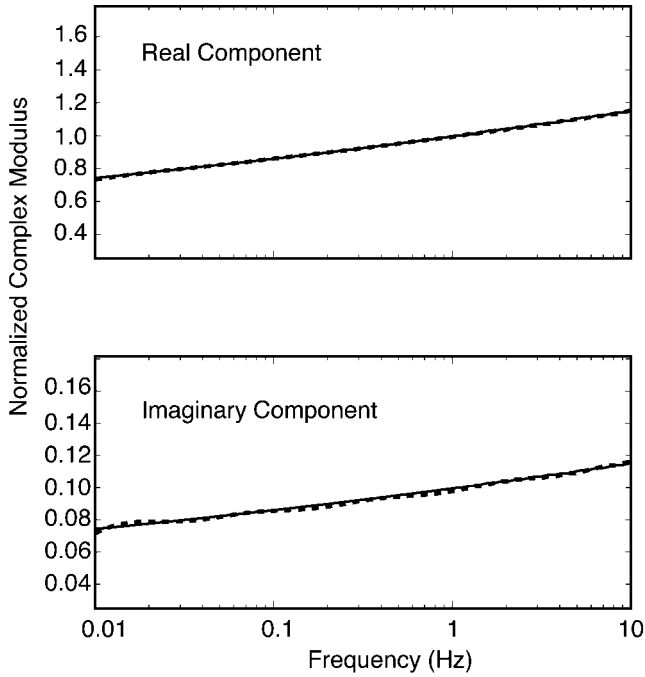


Figure 2. The complex viscoelastic modulus (top, real component; bottom, imaginary component) are plotted versus frequency. The solid lines are components of the modulus from Kjartansson (1979). Dashed lines are calculated from equation (1). Both moduli are normalized by M_0 with the assumption that the reference frequency is 1 Hz.

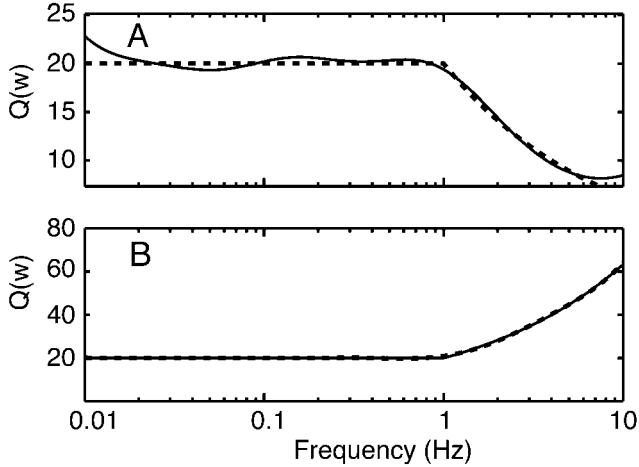


Figure 3. An example showing where the model Q increases (a) or decreases (b) as a function of frequency. The dashed lines are calculated from equation (10). Solid lines are the model results.

greater to accurately model constant Q over three decades in frequency (Emmerich and Korn, 1987; Day and Bradley, 2001). In the next section we derive a formula to calculate the relaxation times τ_k and weight coefficients w_k that can be used in the coarse-grained system devised by Day (1998) to reduce the number of required memory variables.

Modeling Q for Implementing Coarse-Grain Memory Variables

Following the coarse-grained method (Day, 1998; Day and Bradley, 2001), eight pairs of relaxation times and weight coefficients are used to approximate the relaxation functions or Q given by equation (5), but only one pair is assigned to a unit cell of a 3D FD algorithm. So the modulus at a unit cell is expressed as

$$M_k(\omega) = M_u \left(1 - \frac{\bar{w}_k}{1 + i\omega\bar{\tau}_k} \right) \quad (11)$$

In (11), $\bar{\tau}_k$ represents the relaxation time; \bar{w}_k represents the weight coefficient; the subscript k is a number between 1 and 8 that depends on the location (p, q, r) of the unit cell, where p , q , and r are the indices of the cell in the three directions of FD system, respectively. Day (1998) gives a simple formula to determine the practical value of k , that is $k = 1 + (p \bmod 2) + 2(q \bmod 2) + 4(r \bmod 2)$. Similar to equation (2), stress at the cell is given by

$$\sigma(t) = M_u[\varepsilon(t) - \bar{\zeta}_k]. \quad (12)$$

The solution of memory variables $\bar{\zeta}_k$ is same as equation (4) for ζ_k , but with $\bar{\tau}_k$ and \bar{w}_k replacing τ_k and w_k :

$$\begin{aligned} \bar{\zeta}_k(t + \Delta t/2) = & \exp(-\Delta t/\bar{\tau}_k)\bar{\zeta}_k(t - \Delta t/2) \\ & + \bar{w}_k[1 - \exp(-\Delta t/\bar{\tau}_k)]\varepsilon(t). \end{aligned} \quad (13)$$

To determine \bar{w}_k and $\bar{\tau}_k$ used in equations (11) and (13), we need the average modulus over the coarse-grained volume that contains eight adjacent unit cells (3D case). In the conventional coarse-grained method, the average modulus is calculated by equation (1). As noted by Graves and Day (2003), however, the harmonic average of the modulus works better for the coarse-grain system. Following the work of Graves and Day (2003), we express the average modulus over the coarse-grained volume as

$$\overline{M(\omega)} = 8 \left\{ \sum_{k=1}^8 \frac{1}{M_k(\omega)} \right\}^{-1}, \quad (14a)$$

or

$$\overline{M(\omega)} = 8M_u \left\{ \sum_{k=1}^8 \left(\frac{a_k}{a_k^2 + b_k^2} - i \frac{b_k}{a_k^2 + b_k^2} \right) \right\}^{-1}, \quad (14b)$$

where

$$a_k = 1 - \frac{\bar{w}_k}{1 + \omega^2\bar{w}_k^2}, \quad b_k = 1 - \frac{\omega\bar{\tau}_k\bar{w}_k}{1 + \omega^2\bar{w}_k^2} \quad (14c)$$

Given the modulus $\overline{M(\omega_r)} = c^2\rho$ and the preceding equa-

tions, a formula similar to equation (9) can be easily derived for the calculation of the unrelaxed modulus M_u .

Having the complex average modulus, the corresponding $Q(\omega)$ can be written as

$$Q(\omega) = \frac{\text{Re } \overline{M(\omega)}}{\text{Im } \overline{M(\omega)}} \quad (15)$$

Applying the aforementioned technique, \overline{w}_k and $\overline{\tau}_k$ are then obtained by finding the best fit between the synthetic $Q(\omega)$, given by equation (15), and the target Q . Because most FD or finite-element simulations of wave propagation are limited to low frequencies—in general, less than 2 Hz for 3D problems, we restrict the frequency-independent Q to the range 0.01–10 Hz. Again we set $Q_{\min} = 5$, $Q_{\max} = 5000$. The computed relaxation times $\overline{\tau}_k$ are listed in Table 2. Similar to equation (6), an interpolation formula is found for the calculation of the weight coefficients \overline{w}_k^Q for any Q between Q_{\min} and Q_{\max} , which is also of the form

$$\overline{w}_k^Q = \overline{\chi}(\overline{\chi}\overline{\alpha}_k + \overline{\beta}_k), \quad (16a)$$

where the values of $\overline{\alpha}_k$ and $\overline{\beta}_k$ are listed in Table 2; the factor $\overline{\chi}$ is calculated by

$$\overline{\chi} = \frac{5.649 - 0.477 Q^{-0.53} \ln(Q/5)}{1 + 0.109 Q}, \quad 5 \leq Q \leq 5000. \quad (16b)$$

We have calculated different $Q(\omega)$ values using equations (14) (15) (16) and the values listed in Table 2; the different $Q(\omega)$ values are plotted in Figure 4. The solid lines represent simulations and the dashed lines are targets. Although the $Q(\omega)$ formula (equation 14) derived from the harmonic average modulus is more complex than that given by equation (5), the required weight coefficients are accurately determined through interpolation. Figure 4 shows that each model of $Q(\omega)$ has a very good agreement with its target value over the frequency range 0.01–10 Hz. The largest misfit is less than 6% for any frequency.

Table 2

Coefficients for Modeling Q , Equations (14)–(16)

k	$\overline{\tau}_k$	$\overline{\alpha}_k$	$\overline{\beta}_k$
1	7.95929×10^{-3}	1.89599×10^{-2}	8.50577×10^{-2}
2	7.96067×10^{-3}	1.31638×10^{-2}	1.13676×10^{-1}
3	3.28661×10^{-2}	1.55379×10^{-2}	1.36285×10^{-1}
4	1.38501×10^{-1}	1.57445×10^{-2}	1.43302×10^{-1}
5	5.41466×10^{-1}	2.30073×10^{-2}	1.25200×10^{-1}
6	1.97729	2.09506×10^{-2}	1.43108×10^{-1}
7	12.2426	3.42489×10^{-2}	1.04466×10^{-1}
8	12.2427	2.38454×10^{-2}	1.45809×10^{-1}

Numerical Example

We incorporate the aforementioned technique of modeling Q into a FD algorithm by using the coarse-grained method of Day and Bradley (2001). We demonstrate the modeling accuracy by simulating wave propagation in a 1D earth structure. The FD simulations are compared with the solutions obtained by a frequency wavenumber (FK) method (Zhu and Rivera 2002). We have modified this FK code to use either equation (1) or equation (9) to incorporate Q . Both modified FK methods generate the same solution.

We now compute seismograms using the fourth-order staggered-grid velocity-stress FD method (Liu and Archuleta, 2002) for the same test problem used by Graves and Day (2003) that is now described. A double-couple point source with strike = 90°, dip = 90°, rake = 0°, and a depth of 2 km is specified with a moment-rate function given by

$$\dot{M}(t) = \begin{cases} M_0(1 - \cos(2\pi t/T))/T, & 0 < t < T; \\ 0, & \text{otherwise,} \end{cases} \quad (17)$$

where $T = 0.2$ sec and $M_0 = 10^{16}$ N m. The observation point is located at the surface at a distance of 5 km and at an azimuth of 143°. In our FD calculation, the minimum grid spacing is 0.1 km and the timestep is 0.008 sec. With this grid spacing, the model has five grids per minimum shear wavelength at the upper-frequency limit of 1.0 Hz. The velocity seismograms from FD and FK methods are low-pass

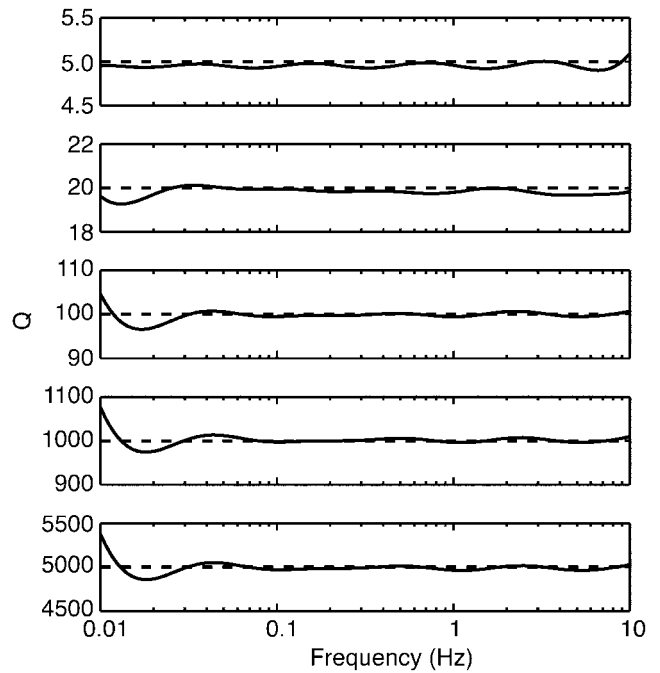


Figure 4. The fit between model Q (solid line) and the target $Q(\omega)$ (dashed line). Model Q is calculated by using equation (15). The relaxation times $\overline{\tau}_k$ or weight coefficients \overline{w}_k are obtained from Table 2 by use of equation (16).

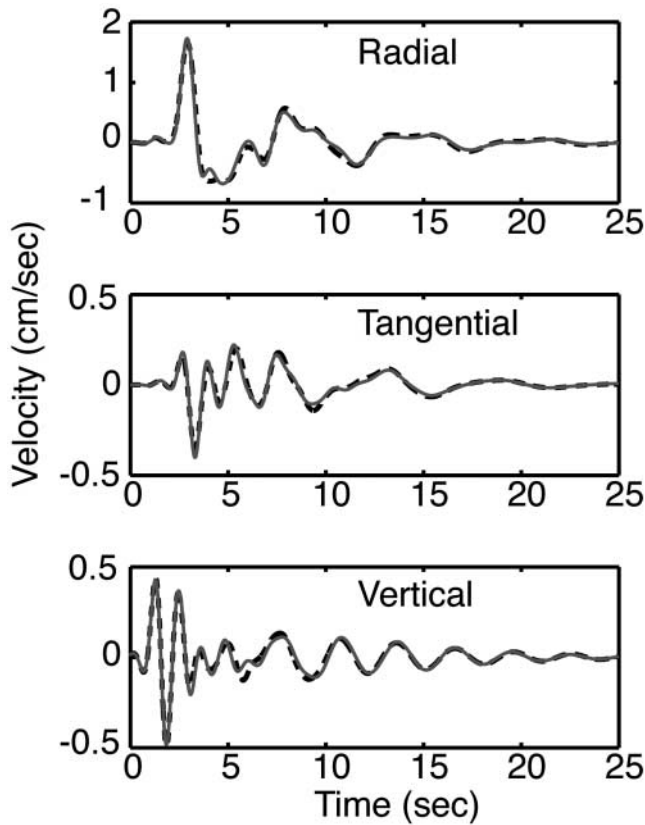


Figure 5. We compare FD (dashed line) and FK (solid line) seismograms for a three-layered Earth model problem (see text). A reference frequency of 1 Hz is used for calculating the unrelaxed modulus. All seismograms are low-pass filtered with a corner frequency of 1 Hz.

filtered with a corner frequency of 1.0 Hz. The seismograms from the FD and FK methods are compared in Figure 5. In the FD simulation, the interfaces of layered velocity structure model at depths 0.55 km and 1.55 km will pass through the grid cell of FD system. The Q -values for these grid cells are determined through interpolation (see Table 3). They are $Q_P = 13.33$ and $Q_S = 6.67$, at a depth of 0.55 km; $Q_P = 33.33$ and $Q_S = 16.67$, at a depth of 1.55 km. The weight coefficients for all Q s, except $Q = 5$, are obtained from equation (16). The excellent agreement between the waveforms shown in Figure 5 demonstrates the accuracy of the modeling of Q by using simple interpolation.

Conclusions

We have developed an approach to determine the relaxation times and weight coefficients required by the widely used Q -modeling methods for time-domain wave propagation (Day and Minster, 1984; Emmerich and Korn, 1987; Blanch *et al.*, 1995; Day and Bradley, 2001). We have also provided two formulas to interpolate the weight coefficients for any Q between 5 and 5000. One is based on an arithmetic

Table 3
Layered Velocity Structure

V_P (km/sec)	V_S (km/sec)	Density (g/cm ³)	Q_P	Q_S	Thickness (km)
1.7	0.5	2.1	10	5	0.55
3.0	1.2	2.3	20	10	1.00
6.0	3.464	2.3	100	50	—

average of the modulus; the other is based on a harmonic average. For each case, one set of relaxation times is given. This technique can properly optimize both weights and relaxation times to model correctly frequency-dependent Q and frequency-independent Q .

We have verified the modeling accuracy of Q by incorporating equation (16) into a FD code that implements the coarse-grained method of Day and Bradley (2001). Our numerical test example confirms that harmonic average moduli, suggested by Graves and Day (2003), works very well to model Q when using a coarse-grained FD method, even for very low Q .

Acknowledgments

This article was improved by careful reviews from Steve Day and Chris Bradley. The research was funded by the USGS Grant under Contract No. 05HQGR0044 and by the Southern California Earthquake Center. SCEC is funded by NSF cooperative Agreement EAR-0106924 and USGS cooperative Agreement 02HQAG0008. This is ICS contribution 720 and SCEC contribution 957.

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Manuscript received 12 August 2005.