Improvement of accuracy of the spectral element method for elastic wave computation using modified numerical integration operators

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Abstract
We introduce new numerical integration operators which compose the mass and stiffness matrices of a modified spectral element method for simulation of elastic wave propagation. While these operators use the same quadrature nodes as does the original spectral element method, they are designed in order that their harmonic responses have errors of the same ratio, and that the respective dispersion errors of the mass and stiffness matrices cancel each other. As a result, the modified spectral element method yields two extra-orders of accuracy, and is comparable to the original method of one order higher. The theoretical results are confirmed by numerical dispersion analysis and examples of computation of waveforms using our operators. Replacing the ordinary operators by those proposed in this study could be a non-expensive solution to improve the accuracy.

Keywords: Elastic wave, FEM, SEM, Error-optimization, Numerical dispersion

1. Introduction

Finite element methods (FEMs) for computation of the elastic wave equation have greatly contributed to revealing rupture process of earthquakes [1], imaging interior structures of the Earth [2], and evaluating seismic hazards [3]. In the above applications, the spectral element method (SEM) is a prominent method [4, 5]. The SEM is a lumped-mass FEM characterized by a high-order quadrature rule with non-equispaced nodal basis functions defined on hexahedral elements, which leads to an explicit time-marching scheme without loss of accuracy of computation. A detailed description is available on [6, 7].

In applications of FEMs to elastic wave computation in complex underground structures, there may still exist difficulty concerning grid-generation. According to dispersion and stability analyses [8–10], it is preferable that the number of spatial grid points vary with the propagation velocities of regions: i.e., in terms of accuracy, the number of grid points per wavelength should be sufficiently large to suppress numerical dispersion [11,12]; conversely, an unnecessarily large number of grid points (or small grid intervals) may increase the total number of time steps as well as computational cost required for each time step, since time intervals should be smaller than the time for a $P$-wave train to pass through one grid interval [11]. Therefore, it is preferable to use almost the same number of grid points per wavelength throughout the medium. However, the rule makes the grid-generation more complicated as velocity structures become complex. Instead of regulating the number of grid points per wavelength, a regional increase of the order of elements would effectively improve the accuracy. However, for the SEM in particular, it is difficult to use elements of heterogeneous orders, without rather complicated implementations [15]. Moreover, a use of higher-order elements can degrade flexibility to match the grid geometry with a model structure, compared with low-order elements with the same number of grid points. Therefore, a superconvergent FEM which
can improve the accuracy without increasing the number and order of elements is highly desired in order to extend FEM applications.

In this paper, we introduce modified numerical integration operators for the SEM for elastic wave computation. While our operators are associated with the same quadrature nodes as those of the SEM, they are designed to yield higher accuracy of computation without increasing the number and order of elements. As a remedy for the above problem, we suggest that a user embed a region of the SEM computation using our operators for desired accuracy, surrounded by regions with the ordinary SEM operators without making any change in grid settings. As another approach related to the above problem, Capdeville et al. [16], Guillot et al. [17], and their series of papers have proposed homogenization of media in order to avoid raw structures with any complexity including irregular boundaries. Our method is also applicable with their approach.

Studies for superconvergent SEM/FEMs are traceable back to the following previous works. Marfurt [18] suppressed the numerical dispersion of the linear FEM by blending the consistent and lumped mass matrices in an empirical way. Seriani and Oliveira [19] extended his study for the SEM. Ainsworth and Wajid [20] analytically found the optimal value of the blending ratio such that the numerical dispersion of the SEM is minimized. Note also that their ideas have been applied to the isogeometric analysis method, which is well-suited for structures with smooth curved surfaces [21–25]. While the above studies are for computation of the Helmholtz equation, an extension to the Maxwell wave equation is given by [26]. In the field of computational seismology, a study for the elastic wave equation is given by [27]. They introduced a general criterion to minimize the modal error based on a perturbation approach, and gave a superconvergent linear FEM for computing elastic wave propagation. In this paper, we begin with a review of the criterion given by [27]. Then, we give modified numerical integration operators which minimize the numerical dispersion of the SEM for the elastic wave computation. Note that our results have some parts related to the optimally blending integration operator previously introduced by [20], which are also derived in this paper in a simpler way. Then, we show some new results for application to the elastic wave computation.

2. Review: general analysis for modal error estimation

While the notations are different from those used in [27], the results in this part have been previously given by [27]. The numerically approximated weak form of the elastic wave equation may be formally written as follows:

$$\omega^2 M^{\text{num}}(\vec{w}, \vec{u}) = K^{\text{num}}(\vec{w}, \vec{u}) - F^{\text{num}}(\vec{w}),$$  \hspace{1cm} (2.1)

where \( \omega \) is the frequency, \( \vec{u} = (u_x, u_y, u_z) \) is the displacement, \( \vec{w} = (w_x, w_y, w_z) \) is the weight function. The numerical operators are given by

$$M^{\text{num}}(\vec{w}, \vec{u}) = \sum_{\alpha=x,y,z} \text{n.i.} \int_V w_\alpha \rho u_\alpha dV \hspace{1cm} (2.2)$$
$$K^{\text{num}}(\vec{w}, \vec{u}) = \sum_{\alpha, \beta, \mu, \nu=x,y,z} \text{n.i.} \int_V \left( \partial_\beta w_\alpha \right) \Gamma_{\alpha\beta\mu\nu} \left( \partial_\nu u_\mu \right) dV \hspace{1cm} (2.3)$$
$$F^{\text{num}}(\vec{w}) = \sum_{\alpha=x,y,z} \text{n.i.} \int_V w_\alpha f_\alpha dV \hspace{1cm} (2.4)$$

where “n.i.” is an abbreviation for “numerical integration” by which the integral is approximated according to a numerical integration rule, \( \alpha, \beta, \mu, \) and \( \nu \) represent dummy indices for \( x, y, \) and \( z \)-axes, \( \partial_\alpha \) denotes partial differentiation with respect to the \( \alpha \)-axis, \( \rho \) is the density, \( \Gamma_{\alpha\beta\mu\nu} \) are the elastic moduli, \( f_\alpha \) is the external body force, and \( V \) denotes the volume of the medium. We denote the exact operators corresponding to \( M^{\text{num}}, K^{\text{num}}, \) and \( F^{\text{num}} \) by \( M, K, \) and \( F, \) respectively, where

$$M(\vec{w}, \vec{u}) = \sum_{\alpha=x,y,z} \int_V w_\alpha \rho u_\alpha dV \hspace{1cm} (2.5)$$
\begin{align}
K(\vec{w}, \vec{u}) &= \sum_{\alpha, \beta, \mu, \nu = x, y, z} \int_V (\partial_\beta w_\alpha) \Gamma_{\alpha \beta \mu \nu} (\partial_\nu u_\mu) dV \\
F(\vec{w}) &= \sum_{\alpha = x, y, z} \int_V w_\alpha f_\alpha dV.
\end{align}

Herein, we consider the case for \( f_\alpha = 0 \). In this case, Eq. (2.1) becomes the following eigenvalue problem:
\begin{equation}
K_{\text{num}}(\vec{w}, \vec{u}_{\text{num} i}) = (\omega_{\text{num} i})^2 M_{\text{num}}(\vec{w}, \vec{u}_{\text{num} i}),
\end{equation}
where \( \omega_{\text{num} i} \) and \( \vec{u}_{\text{num} i} \) are the numerical eigenfrequency and eigenvector of the \( i \)-th mode, respectively. The numerical eigenvectors are orthonormalized as follows:
\begin{equation}
M_{\text{num}}([\vec{u}_{\text{num} i}]^* , \vec{u}_{\text{num} j}) = \delta_{ij},
\end{equation}
where the asterisk indicates complex conjugate, and \( \delta_{ij} \) is the Kronecker-delta. Similarly, the eigenvalue problem for the exact operators is
\begin{equation}
K(\vec{w}, \vec{u}_i) = \omega_i^2 M(\vec{w}, \vec{u}_i),
\end{equation}
where \( \omega_i \) and \( \vec{u}_i \) are the exact eigenfrequency and eigenvector of the \( i \)-th mode, respectively. The exact eigenvectors are orthonormalized as follows:
\begin{equation}
M ([\vec{u}_i]^* , \vec{u}_j) = \delta_{ij}.
\end{equation}

We formally denote the error of the numerical operators by \( \delta M \) and \( \delta K \), and the error of the numerical eigenfrequency and eigenvector of the \( i \)-th mode by \( \delta \omega_i \) and \( \delta \vec{u}_i \), where
\begin{align}
M_{\text{num}}(\vec{w}, \vec{v}) &= M(\vec{w}, \vec{v}) + \delta M(\vec{w}, \vec{v}) \\
K_{\text{num}}(\vec{w}, \vec{v}) &= K(\vec{w}, \vec{v}) + \delta K(\vec{w}, \vec{v}) \\
\omega_{\text{num} i} &= \omega_i + \delta \omega_i \\
\vec{u}_{\text{num} i} &= \vec{u}_i + \delta \vec{u}_i,
\end{align}
where \( \vec{w} = (w_x, w_y, w_z) \) and \( \vec{v} = (v_x, v_y, v_z) \) are arbitrary functions. Substituting Eqs. (2.12)–(2.15) into Eq. (2.8) for the case of \( \vec{w} = \vec{u}_i \), and taking the first-order perturbation with some algebra, The error of the numerical eigenfrequency is approximated as follows:
\begin{equation}
\delta \omega_i \approx \frac{\delta K ([\vec{u}_i]^* , \vec{u}_i) - \omega_i^2 \delta M ([\vec{u}_i]^* , \vec{u}_i)}{2 \omega_i}.
\end{equation}
Consequently, we have \( \delta \omega_i = 0 \) when the numerical operators approximately satisfy
\begin{equation}
\delta K ([\vec{u}_i]^* , \vec{u}_i) \approx \omega_i^2 \delta M ([\vec{u}_i]^* , \vec{u}_i).
\end{equation}
Dividing Eq. (2.17) by Eq. (2.10) with \( \vec{w} = [\vec{u}_i]^* \), Eq. (2.17) can be rewritten as follows:
\begin{equation}
\frac{\delta M ([\vec{u}_i]^* , \vec{u}_i)}{M ([\vec{u}_i]^* , \vec{u}_i)} \approx \frac{\delta K ([\vec{u}_i]^* , \vec{u}_i)}{K ([\vec{u}_i]^* , \vec{u}_i)}.
\end{equation}
In other words, the error of the numerical eigenfrequency will be minimized when the numerical operators have modal errors of the same ratio.
3. Numerical integration operators

We consider a FEM such that the global operators $M^{\text{num}}$ and $K^{\text{num}}$ of Eqs. (2.2) and (2.3) can be written as the superposition of local operators for respective elements, as in the SEM. If the local operators for each element satisfy Eq. (2.17), so will the global operators. Hence, this argument can proceed with a focus on a single element.

To simplify the problem, we consider the regular Cartesian grid with $\Delta x = \Delta y = \Delta z$, and ignore effects of element distortion. Furthermore, we assume that the medium can be regarded as homogeneous on a local scale comparable to the element size, and there is no boundary in the vicinity of the element on which we focus. Note that these assumptions are commonly used in measurement of numerical dispersion [10–14]. Indeed, the error of the numerical eigenfrequency of Eq. (2.8) is exactly equivalent to the definition of the numerical dispersion when we consider the case of an unbounded and homogeneous medium. Therefore, our objective is to derive operators which minimize the numerical dispersion. On these assumptions, plane waves can be used for the modes in the vicinity of the element we focus on: $\vec{u}_j(\vec{x}) = \vec{E}^\gamma e^{i\vec{k}\cdot\vec{x}} = \vec{E}^\gamma p_k(x)p_k(y)p_k(z), \quad (3.1)$

where $i$ is the imaginary unit, $e$ is the Napier’s constant, $k = (k_x, k_y, k_z)$ denotes the wavenumber vector, $\vec{x} = (x, y, z)$ denotes the Cartesian coordinate, $\gamma$ specifies the type of polarization (i.e. $P$ and $S$-waves), $\vec{E}^\gamma = (E^\gamma_x, E^\gamma_y, E^\gamma_z)$ denotes the amplitude vector, $j$ is the pointer to $(\gamma, \vec{k})$, and $p_k$ denotes the imaginary exponential function with wavenumber $k$: $p_k(x) = e^{ikx}. \quad (3.2)$

Note that $\vec{E}^\gamma$ is parallel to $\vec{k}$ when $\gamma$ specifies the $P$-wave, or perpendicular to $\vec{k}$ when $\gamma$ specifies the $S$-wave.

We define the following three types of numerical integration operators: $A^{\text{num}}(\phi, \psi) = \text{n.i.} \int_{-h/2}^{h/2} \phi \psi dx \quad (3.3)$

$B^{\text{num}}(\phi, \psi) = \text{n.i.} \int_{-h/2}^{h/2} \phi' \psi' dx \quad (3.4)$

$C^{\text{num}}(\phi, \psi) = \text{n.i.} \int_{-h/2}^{h/2} \phi' \psi dx \quad (3.5)$

where “n.i.” is used for the same meaning as Eqs. (2.2)–(2.4), $\phi$ and $\psi$ are arbitrary functions of $x$, “$'$” denotes the spatial differentiation, and $h$ denotes the length of the element. We here suppose that $M^{\text{num}}$ and $K^{\text{num}}$ can be expressed in terms of tensor products of the above integration operators for the $x$, $y$, and $z$-axes, as in the SEM. Then, noting that the plane waves (3.1) are expressed as the products of imaginary exponential functions for the $x$, $y$, and $z$-axes, $M^{\text{num}}(\vec{u}_i^\gamma, \vec{u}_j^\gamma)$ and $K^{\text{num}}(\vec{u}_i^\gamma, \vec{u}_j^\gamma)$ can be expressed in terms of products of the harmonic responses of the integration operators, $A^{\text{num}}(p_k^\gamma, p_k^\gamma)$, $B^{\text{num}}(p_k^\gamma, p_k^\gamma)$, and $C^{\text{num}}(p_k^\gamma, p_k^\gamma)$ with $k = k_x, k_y, k_z$. Therefore, Eq. (2.17) can be simply decomposed into the following conditions for the integration operators: $\frac{\delta A(p_k^\gamma, p_k^\gamma)}{A(p_k^\gamma, p_k^\gamma)} \approx \frac{\delta B(p_k^\gamma, p_k^\gamma)}{B(p_k^\gamma, p_k^\gamma)} \approx \frac{\delta C(p_k^\gamma, p_k^\gamma)}{C(p_k^\gamma, p_k^\gamma)}, \quad (3.6)$

where $A$, $B$, and $C$ are the exact integration operators corresponding to $A^{\text{num}}$, $B^{\text{num}}$, and $C^{\text{num}}$, respectively, and $\delta A$, $\delta B$, and $\delta C$ are the errors, where

$A^{\text{num}}(\phi, \psi) = A(\phi, \psi) + \delta A(\phi, \psi) \quad (3.7)$

$B^{\text{num}}(\phi, \psi) = B(\phi, \psi) + \delta B(\phi, \psi) \quad (3.8)$

$C^{\text{num}}(\phi, \psi) = C(\phi, \psi) + \delta C(\phi, \psi). \quad (3.9)$
As indicated by Eq. (2.18) for this case, the numerical dispersion will be suppressed when $M^{\text{num}}$ and $K^{\text{num}}$ have dispersion errors of the same ratio. Then, since they are based on the integration operators Eqs. (3.3)–(3.5), they will have the dispersion errors of the same ratio when the harmonic responses of the integration operators have errors of the same ratio.

We note that there is no other measure to define the scale of space than the length of the element $h$ and wavelength $\lambda = 2\pi/k$, i.e., to increase the wavelength is to decrease the element size. Therefore, hereafter in this section, we can fix the absolute value of $h$ as $h = 2$ without loss of generality, and we introduce the following normalized length instead of the actual length of the element:

$$\hat{h} = \pi h/\lambda (= k).$$

(3.10)

If necessary, the reader can proceed following discussions for general cases of arbitrary values of $h$, by multiplying the integrals (3.3)-(3.5) with $h = 2$ by factors of $h/2$, $2/h$, and 1, respectively, and by replacing $\phi(x)$ and $\psi(x)$ with $\phi(hx/2)$ and $\psi(hx/2)$.

### 3.1. SEM integration operators

We denote numerical operators $A^{\text{num}}$, $B^{\text{num}}$, and $C^{\text{num}}$ defined based on the SEM by $A^{\text{SEM}}$, $B^{\text{SEM}}$, and $C^{\text{SEM}}$, respectively. For the case of the SEM, the operands of Eqs. (3.3)–(3.5) are approximated as follows:

$$\phi(x) \approx \sum_{i=0}^{n} \phi(x_i)L_i(x)$$

(3.11)

$$\psi(x) \approx \sum_{i=0}^{n} \psi(x_i)L_i(x),$$

(3.12)

where $n$ is the degree of the polynomial (i.e. the order of elements), $x_i$ are the Gauss-Lobatto-Legendre (GLL) nodes in ascending order as increasing number $i = 0, \ldots, n$ as follows:

$$x_0 = -1 < x_1 < \ldots < x_{n-1} < x_n = 1.$$  

(3.13)

$L_i$ are Lagrange interpolating polynomials defined as

$$L_i(x) = \prod_{j=0, j\neq i}^{n} \frac{x - x_j}{x_i - x_j}.$$  

(3.14)

Then, the SEM integration operators are defined based on the GLL quadrature rule as follows:

$$A^{\text{SEM}}(\phi, \psi) = \sum_{i,j=0}^{n} \phi(x_i)\psi(x_j) \int_{-1}^{1} L_i L_j dx$$

(3.15)

$$= \sum_{i=0}^{n} \phi_i q_i \psi_i,$$

$$B^{\text{SEM}}(\phi, \psi) = \sum_{i,j=0}^{n} \phi(x_i)\psi(x_j) \int_{-1}^{1} L'_i L'_j dx$$

(3.16)

$$= \sum_{m=0}^{n} \left[ \sum_{i=0}^{n} D_{mi} \phi_i \right] q_m \left[ \sum_{j=0}^{n} D_{mj} \psi_j \right]$$

$$C^{\text{SEM}}(\phi, \psi) = \sum_{i,j=0}^{n} \phi(x_i)\psi(x_j) \int_{-1}^{1} L'_i L_j dx$$

(3.17)

$$= \sum_{i,j=0}^{n} D_{ji} \phi_i q_j \psi_j.$$
where \( \phi_i = \phi(x_i) \), \( \psi_i = \psi(x_i) \), \( q_i \) are the GLL weights, and

\[ D_{ij} = L_j'(x_i). \]  
(3.18)

An explicit form of \( L_j'(x_i) \) is given by Eq. (A.20) in Appendix A. Note that the integral in Eq. (3.15) is approximated based on the GLL rule, whereas those in Eqs. (3.16) and (3.17) are exactly calculated, since the GLL rule exactly computes an integral when the integrand is a polynomial of degree \( (2n - 1) \) or below.

For the exact operators, we have

\[
A(p_i^*, p_h) = \int_{-1}^{1} \left| p_h(x) \right|^2 dx = 2 
\]  
(3.19)

\[
B(p_i^*, p_h) = \int_{-1}^{1} \left| p_h'(x) \right|^2 dx = 2\hat{h}^2 
\]  
(3.20)

\[
C(p_i^*, p_h) = \int_{-1}^{1} p_h(x)^* p_h(x) dx = -2i\hat{h}. 
\]  
(3.21)

Substituting \((p_i^*, p_h)\) into \((\phi, \psi)\) of Eqs. (3.15)–(3.17), respectively, and comparing them with the exact results (3.19)–(3.21), the relative response errors are given by

\[
\delta A_{SEM}(p_i^*, p_h) = 0 
\]  
(3.22)

\[
\delta B_{SEM}(p_i^*, p_h) = \mathcal{E}_n \hat{h}^{2n} + O(\hat{h}^{2n+2}) 
\]  
(3.23)

\[
\delta C_{SEM}(p_i^*, p_h) = (n+1)\mathcal{E}_n \hat{h}^{2n} + O(\hat{h}^{2n+1}) 
\]  
(3.24)

where \( O(\hat{h}^l) \) represents terms having \( \hat{h} \) to the power of \( l \) or above, and \( \mathcal{E}_n \) is given by

\[
\mathcal{E}_n = -\frac{n}{4(2n+1)(n!)^2} \left[ \sum_{i=0}^{n} q_i P_n(x_i) x_i^n \right]^2, 
\]  
(3.25)

where \( P_n \) is the Legendre polynomial of the \( n \)-th-order. In Appendix B we show algebra for their derivations.

Comparing Eqs. (3.22)–(3.24), we obviously see that their \( 2n \)-th-order terms are different from each other, and thus the SEM operators (3.15)–(3.17) do not satisfy Eq. (3.6) at the \( 2n \)-th-order.

### 3.2. Modified integration operators

Hereafter, we denote numerical operators \( A^{num} \), \( B^{num} \), and \( C^{num} \) such that they satisfy Eq. (3.6) by \( A^{opt} \), \( B^{opt} \), and \( C^{opt} \), respectively. Firstly, we assume that \( B^{opt} \) is simply given by

\[
B^{opt}(\phi, \psi) = B^{SEM}(\phi, \psi), 
\]  
(3.26)

and then we define \( A^{opt} \) and \( C^{opt} \) such that their response errors have the same ratio as Eq. (3.23). Note that in this paper we propose one solution, while there could be other ways of modification which satisfy Eq. (3.6), but do not assume Eq. (3.26). The starting point is exactly same as the mass-blending approaches (e.g. [18][20]).

In order to define \( A^{opt} \), we make another FEM definition for \( A^{num} \) such that we compute the integral in Eq. (3.15) exactly as follows:

\[
A^{FEM}(\phi, \psi) = \sum_{i,j=0}^{n} \phi_i \psi_j \int_{-1}^{1} L_i L_j dx 
\]  

\[
= A^{SEM}(\phi, \psi) - \frac{n(n+1)}{2(2n+1)} \left[ \sum_{i=0}^{n} \phi_i q_i P_n(x_i) \right] \left[ \sum_{j=0}^{n} \psi_j q_j P_n(x_j) \right], 
\]  
(3.27)
where $A^{SEM}$ represents the second line of Eq. (3.15). The algebra for calculation of the integral in Eq. (3.27) is shown in Eq. (A.24) in Appendix A. The relative response error of $A^{FEM}$ is given by

$$
\frac{\delta A^{FEM}(p^*, p_h)}{A(p^*_h, p_h)} = (n + 1)\xi^2_n h^{2n} + O(h^{2n+2}).
$$

(3.28)

The derivation is shown in Appendix B (see eq. B.2).

We define $A^{opt}$ by blending $A^{SEM}$ and $A^{FEM}$ of Eqs. (3.15) and (3.27). Since the error of $A^{opt}$ is also linearly controlled by its blending ratio, we immediately obtain the optimal ratio such that the error is equal to Eq. (3.23) as follows:

$$
A^{opt}(\phi, \psi) = \frac{n}{n+1} A^{SEM}(\phi, \psi) + \frac{1}{n+1} A^{FEM}(\phi, \psi)
$$

(3.29)

$$
= A^{SEM}(\phi, \psi) - \frac{n}{2(2n+1)} \left[ \sum_{i=0}^{n} \phi_i q_i P_n(x_i) \right] \left[ \sum_{j=0}^{n} \psi_j q_j P_n(x_j) \right].
$$

Note that the blending approach itself has already been reported by previous papers, and the optimal value of blending ratio has been analytically given by \[20\]. Eq. (3.29) follows their result, except for differences in the derivation.

To define $C^{opt}$, we make the following approximation for the operand $\phi$, instead of Eq. (3.11):

$$
\phi(x) \approx \sum_{i=-1}^{n} \phi(x_i) X_i(x),
$$

(3.30)

where $X_i$ are Lagrange interpolating polynomials of degree $(n + 1)$ defined as follows:

$$
X_i(x) = \prod_{j=-1, j \neq i}^{n} \frac{x - x_j}{x_i - x_j}.
$$

(3.31)

Note that the product is taken for $j$ from $-1$ to $n$ except $j = i$. $x_i$ denote the GLL nodes (3.13) except for the case of $i = -1$: $x_{-1}$ is an arbitrary node other than $x_0, x_1, \ldots, x_n$. In this paper, we define $x_{-1}$ as follows:

$$
x_{-1} = x_{n-1} - 2.
$$

(3.32)

The definition (3.32) indicates that $x_{-1}$ is located next to the left of $x_0$, when we take the positive direction to the right of the $x$-axis. Consequently, we use a node outside the domain of the integration for computation of Eq. (3.5). Note that, by the definition, the approximation (3.30) cannot be used when the domain is located on the leftmost of a medium. We can use a node on the right side for that case, or we may simply use the ordinary SEM operator $C^{SEM}$ only for that case. We use the approximation of Eq. (3.12) for the operand $\psi$. Then, we define $C^{opt}$ as follows:

$$
C^{opt}(\phi, \psi) = \sum_{i=-1, j=0}^{n} \phi_i \psi_j \int_{-1}^{1} X_i L_j dx
$$

$$
= C^{SEM}(\phi, \psi)
$$

$$
+ \frac{n^2(n + 1)}{2(2n+1)} \left[ \sum_{i=0}^{n} \phi_i q_i P_n(x_i) \frac{2\phi_{-1}}{(x_{-1}^2 - 1) P''_n(x_{-1})} \right] \left[ \sum_{j=0}^{n} \psi_j q_j P_n(x_j) \right].
$$

(3.33)

where $\phi_{-1} = \phi(x_{-1})$. The algebra for calculation of the integral in Eq. (3.33) is shown in Eqs. (A.26) and (A.27) in Appendix A.
The relative response errors of the modified numerical operators are given by

$$\frac{\delta A^\text{opt}(p^*_n, p^*_h)}{A(p^*_n, p^*_h)} = \mathcal{E}_n \hat{h}^{2n} + O(\hat{h}^{2n+2})$$  \hspace{1cm} (3.34)

$$\frac{\delta B^\text{opt}(p^*_n, p^*_h)}{B(p^*_n, p^*_h)} = \mathcal{E}_n \hat{h}^{2n} + O(\hat{h}^{2n+2})$$  \hspace{1cm} (3.35)

$$\frac{\delta C^\text{opt}(p^*_n, p^*_h)}{C(p^*_n, p^*_h)} = \mathcal{E}_n \hat{h}^{2n} + O(\hat{h}^{2n+1}).$$  \hspace{1cm} (3.36)

Their derivations are shown in Appendix B. Comparing Eqs. (3.34)–(3.36), we obviously see that the relative response error of \(C^\text{opt}\) may have a non-zero pure imaginary term at the \((2n+1)\)-th-order. Nevertheless, \(\delta K([\vec{u}]^*, \vec{u})\) will not be affected by the imaginary error regardless of its value, since it is canceled out with its complex conjugate when we construct \(K^\text{num}([\vec{u}]^*, \vec{u})\). Consequently, the modified operators will satisfy Eq. (2.17) and then (2.18) up to the \((2n+1)\)-th-order.

3.2.1. Cases of heterogeneous media

We extend the above derivation to general heterogeneous media. Eqs. (2.2) and (2.3) can be expressed in terms of tensor products of the following numerical integration operators:

$$A^\text{num}(\phi, Z, \psi) = \text{n.i.} \int_{-h/2}^{h/2} \phi Z \psi \, dx$$  \hspace{1cm} (3.37)

$$B^\text{num}(\phi, Z, \psi) = \text{n.i.} \int_{-h/2}^{h/2} \phi' Z \psi' \, dx$$  \hspace{1cm} (3.38)

$$C^\text{num}(\phi, Z, \psi) = \text{n.i.} \int_{-h/2}^{h/2} \phi' Z \psi \, dx,$$  \hspace{1cm} (3.39)

where \(\phi, \psi, \text{ and } Z\) are arbitrary functions of \(x\). For simplicity, we continue considering the case for \(h = 2\). Eqs. (3.29) and (3.33) are also applicable for heterogeneous cases by replacing the operand \(\psi\) by \(Z\psi\); i.e., we define \(A^\text{opt}\) and \(C^\text{opt}\) for heterogeneous cases as follows:

$$A^\text{opt}(\phi, Z, \psi) = \sum_{i=0}^{n} \phi_i q_i Z_i \psi_i - \frac{n}{2(2n+1)} \sum_{i=0}^{n} \phi_i q_i P_n(x_i) \left[ \sum_{j=0}^{n} Z_j \psi_j q_j P_n(x_j) \right]$$  \hspace{1cm} (3.40)

$$C^\text{opt}(\phi, Z, \psi) = \sum_{i,j=0}^{n} D_{ij} \phi_i q_j Z_j \psi_j + \frac{n^2(n+1)}{2(2n+1)} \sum_{i=0}^{n} \phi_i q_i P_n(x_i) + \frac{2\phi_{n-1}}{(x_{n-1}^2 - 1) P_n'(x_{n-1})} \left[ \sum_{j=0}^{n} Z_j \psi_j q_j P_n(x_j) \right],$$  \hspace{1cm} (3.41)

where \(Z_i = Z(x_i)\). For \(B^\text{opt}\), we use the ordinary SEM integration operator for heterogeneous cases:

$$B^\text{opt}(\phi, Z, \psi) = \sum_{i,j=0}^{n} \phi_i \psi_j \int_{-1}^{1} L_i' Z L_j' \, dx$$

$$\approx \sum_{m=0}^{n} \left[ \sum_{i=0}^{n} D_{mi} \phi_i \right] Z_m q_m \left[ \sum_{j=0}^{n} D_{mj} \psi_j \right],$$  \hspace{1cm} (3.42)
where we use the GLL rule for the approximation for the integral in Eq. (3.42). Note that when $Z$ is independent of $x$ (i.e. the homogeneous case), Eqs. (3.40)–(3.42) are obviously equal to Eqs. (3.29), (3.33), and (3.16) with multiplying the constant $Z$, respectively. Unfortunately, for heterogeneous cases, it would be difficult to theoretically probe effectiveness of substituting the modified operators for the SEM operators. Instead, in Section 5, we show some examples of numerical computation using our method for a heterogeneous case.

4. Volumetric integration

Before proceeding with this section, we express $A^{opt}$, $B^{opt}$, and $C^{opt}$ in terms of matrix products as follows:

$$A^{opt} = \sum_{i,j} \phi_i A^{opt}_{ij} \psi_j$$

$$B^{opt} = \sum_{i,j} \phi_i B^{opt}_{ij} \psi_j$$

$$C^{opt} = \sum_{i=-1,j=0} \phi_i C^{opt}_{ij} \psi_1,$$

where $\phi_i$, $\phi_2$ and $\psi$ are

$$\phi_1 = [\phi_0, \ldots, \phi_n]^T, \quad \phi_2 = [\phi_{-1}, \phi_0, \ldots, \phi_n]^T, \quad \psi = [\psi_0, \ldots, \psi_n]^T.$$ 

Note that the size of $A^{opt}$ and $B^{opt}$ is $n \times n$, whereas the size of $C^{opt}$ is $(n+1) \times n$. The components of the matrices are

$$A^{opt}_{ij} = A^{opt}(L_i, L_j) = q_i \delta_{ij} - \frac{n}{2(2n+1)} q_i P_n(x_i) q_j P_n(x_j)$$

$$B^{opt}_{ij} = B^{opt}(L_i, L_j) = \sum_{m=0}^n D_m q_m D_{mj}$$

$$C^{opt}_{ij} = C^{opt}(X_i, L_j) = \begin{cases} 
D_j q_j + \frac{n^2(n+1)}{2(2n+1)} q_j P_n(x_i) q_j P_n(x_j) & \text{if } i \neq -1 \\
\frac{n^2(n+1)}{2n+1} \frac{q_j P_n(x_j)}{(x_{i-1}^2 - 1) P_n'(x_{i-1})} & \text{if } i = -1 
\end{cases}$$

where $i, j = 0, \ldots, n$, except for Eq. (4.7); in that case, we consider $i = -1, 0, \ldots, n$.

Since Eqs. (2.2) and (2.3) are rather complex, full-derivation of their explicit formulas is tedious. Instead, we consider the following examples for 2-D volume integrals:

$$I_1(w, u) = \int_{-h/2}^{h/2} \int_{-h/2}^{h/2} w \Gamma u dxdy$$

$$I_2(w, u) = \int_{-h/2}^{h/2} \int_{-h/2}^{h/2} (\partial_x w) \Gamma (\partial_x u) dxdy$$

$$I_3(w, u) = \int_{-h/2}^{h/2} \int_{-h/2}^{h/2} (\partial_y w) \Gamma (\partial_y u) dxdy,$$

where $w, u$ and $\Gamma$ are functions of $(x, y)$. Herein, we approximate these integrals by using the numerical integration operators defined in Section 3.2. By using a similar way to the following description for the
Similarly, substituting Eqs. (4.11) and (4.12) into Eq. (4.9), we can straightforwardly construct the explicit formulas for operators (2.2) and (2.3) for the 2-D/3-D volume.

First, we consider the case that $\Gamma$ is a constant. For the integration of Eq. (4.8), we approximate $w$ and $u$ as follows:

\[ w(x, y) \approx \sum_{i_x, i_y=0}^{n} w_{(i_x, i_y)} L_{i_x}(\hat{x}) L_{i_y}(\hat{y}) \quad (4.11) \]
\[ u(x, y) \approx \sum_{i_x, i_y=0}^{n} u_{(i_x, i_y)} L_{i_x}(\hat{x}) L_{i_y}(\hat{y}), \quad (4.12) \]

where $x = h\hat{x}/2$ and $y = h\hat{y}/2$, and

\[ w_{(i_x, i_y)} = w(hx_{i_x}/2, hx_{i_y}/2) \quad (4.13) \]
\[ u_{(i_x, i_y)} = u(hx_{i_x}/2, hx_{i_y}/2). \quad (4.14) \]

Note that $x_i (i = 0, \ldots, n)$ denote the GLL nodes (3.13). Substituting Eqs. (4.11) and (4.12) into Eq. (4.8), we have

\[ I_1(w, u) \approx \left(\frac{h}{2}\right)^2 \sum_{i_x, i_y=0}^{n} \sum_{j_x, j_y=0}^{n} w_{(i_x, i_y)} \Gamma u_{(j_x, j_y)} \int_{-1}^{1} L_{i_x} L_{j_x} d\hat{x} \int_{-1}^{1} L_{i_y} L_{j_y} d\hat{y} \]
\[ \approx \left(\frac{h}{2}\right)^2 \sum_{i_x, i_y=0}^{n} \sum_{j_x, j_y=0}^{n} w_{(i_x, i_y)} \Gamma u_{(j_x, j_y)} A_{i_x,j_x}^{\text{opt}} A_{i_y,j_y}^{\text{opt}}. \quad (4.15) \]

Similarly, substituting Eqs. (4.11) and (4.12) into Eq. (4.9), $I_2$ is approximated as follows:

\[ I_2(w, u) \approx \sum_{i_x, i_y=0}^{n} \sum_{j_x, j_y=0}^{n} w_{(i_x, i_y)} \Gamma u_{(j_x, j_y)} \int_{-1}^{1} L_{i_x} L_{j_x} d\hat{x} \int_{-1}^{1} L_{i_y} L_{j_y} d\hat{y} \]
\[ \approx \sum_{i_x, i_y=0}^{n} \sum_{j_x, j_y=0}^{n} w_{(i_x, i_y)} \Gamma u_{(j_x, j_y)} B_{i_x,j_x}^{\text{opt}} A_{i_y,j_y}^{\text{opt}}. \quad (4.16) \]

For the integration of Eq. (4.10), we use the following approximation for $w$ and $u$:

\[ w(x, y) \approx \sum_{i_x=-1}^{n} w_{(i_x, i_y)} X_{i_x}(\hat{x}) L_{i_y}(\hat{y}) \quad (4.17) \]
\[ u(x, y) \approx \sum_{i_x=-1}^{n} u_{(i_x, i_y)} L_{i_x}(\hat{x}) X_{i_y}(\hat{y}), \quad (4.18) \]

where $w_{(i_x, i_y)}$ and $u_{(i_x, i_y)}$ are given by Eqs. (4.13) and (4.14), except that $i_x$ of Eq. (4.17) and $i_y$ of Eq. (4.18) represent integers from $-1$ to $n$. Substituting Eqs. (4.17) and (4.18) into Eq. (4.10), $I_3$ is approximated as follows:

\[ I_3(w, u) \approx \sum_{i_x=-1}^{n} \sum_{i_y=0}^{n} w_{(i_x, i_y)} \Gamma u_{(j_x, j_y)} \int_{-1}^{1} X'_{i_x} L_{j_x} d\hat{x} \int_{-1}^{1} L_{i_y} X'_{j_y} d\hat{y} \]
\[ \approx \sum_{i_x=-1}^{n} \sum_{i_y=0}^{n} w_{(i_x, i_y)} \Gamma u_{(j_x, j_y)} C_{i_x,j_x}^{\text{opt}} C_{j_y}^{\text{opt}}. \quad (4.19) \]

For general cases in which $\Gamma$ is a function of $(x, y)$, we approximate $\Gamma$ as follows:

\[ \Gamma(x, y) \approx \sum_{i_x, i_y=0}^{n} \Gamma_{(i_x, i_y)} L_{i_x}(\hat{x}) L_{i_y}(\hat{y}), \quad (4.20) \]
where
\[ \Gamma_{(x_0, y_0)} = \Gamma(hx_{x_0}/2, hx_{y_0}/2). \]  
(4.21)

By using a similar way to the case of a constant \( \Gamma \), we approximate \( I_1, I_2, \) and \( I_3 \) as follows:

\[ I_1(w, u) \approx \left( \frac{h}{2} \right)^2 \sum_{x_{x_0}=0}^{n} \sum_{j_{j_0}=0}^{n} w(x_{x_0}, j_{j_0}) \Gamma_{(j_{j_0}, y_{j_0})} u_{j_{j_0}} A_{x_{x_0} j_{j_0}} A_{x_{x_0} j_{j_0} y_{j_0}} \]  
(4.22)

\[ I_2(w, u) \approx \sum_{x_{x_0}=0}^{n} \sum_{j_{j_0}=0}^{n} w(x_{x_0}, j_{j_0}) \Gamma_{(j_{j_0}, y_{j_0})} u_{j_{j_0}} D_{x_{x_0}} q_{x_{x_0}} D_{x_{x_0} j_{j_0}} A_{x_{x_0} j_{j_0} y_{j_0}} \]  
(4.23)

\[ I_3(w, u) \approx \sum_{x_{x_0}=-1, j_{j_0}=0}^{n} \sum_{j_{j_0}}^{n} w(x_{x_0}, j_{j_0}) \Gamma_{(j_{j_0}, y_{j_0})} u_{j_{j_0}} C_{x_{x_0} j_{j_0}} C_{x_{x_0} j_{j_0} y_{j_0}} \]  
(4.24)

For their derivations we use the following approximations:

\[ \int_{-1}^{1} L_i L_m L_j d\hat{x} \approx \delta_{m j} A_{i j}^{opt} \]  
(4.25)

\[ \int_{-1}^{1} L_i^2 L_m L_j d\hat{x} \approx D_{m j} q_{m} D_{m j} \]  
(4.26)

\[ \int_{-1}^{1} X_i L_m L_j d\hat{x} \approx \delta_{m j} C_{i j}^{opt} \]  
(4.27)

where Eqs. (4.25) and (4.26) are obtained from Eqs. (4.40) and (4.42) with \((\phi, Z, \psi) = (L_i, L_m, L_j)\), and Eq. (4.27) from Eq. (3.41) with \((\phi, Z, \psi) = (X_i, L_m, L_j)\).

5. Numerical examples

First, we show the numerical dispersion of our method. Our analysis is based on the Rayleigh quotient approach developed by [12–14, 19], which is a novel method for efficient estimation of the numerical dispersion in a practical range of the number of grid points. Herein, we consider the frequency-domain equation, and the approach developed by [12–14, 19], which is a novel method for efficient estimation of the numerical dispersion properties of our method and the SEM of several orders. The errors are plotted as functions of the average number of grid points per wavelength \( G \). We define \( G \) as follows:

\[ G = \frac{\lambda}{h/n} = \frac{2\pi n}{h|\vec{k}|}, \]  
(5.1)

where \( \lambda \) and \( |\vec{k}| \) denote the wavelength and wavenumber of a plane \( P \) or \( S \)-wave (3.1), and \( (h/n) \) indicates the average of the length between two adjacent grid intervals for the \( x \) and \( y \)-axes. We evaluate the numerical dispersion as follows:

\[ \text{Dispersion} = \frac{\omega_{num} - V_g |\vec{k}|}{V_g |\vec{k}|} \times 100\%, \]  
(5.2)

where \( \omega_{num} \) is the numerical eigenfrequency of Eq. (2.8) that is obtained by the Rayleigh quotient approach, and \( V_g \) represents \( V_P \) or \( V_S \). We see from Fig. 1 that our method has the dispersion error smaller than the SEM of the same order and is comparable to the SEM of one order higher, which follows our theoretical results in Section 3.

Next, we give demonstrations of solving the time-domain equation using our method. Herein, We consider two model structures: (a) homogeneous and (b) vertically (\( y \)-directionally) heterogeneous models. Each
model is a square of 2-D isotropic elastic medium surrounded by free-surface boundaries with the size 1000 km × 1000 km. As shown in Fig. 2, a source and receiver are located at (300 km, 300 km) and (700 km, 1000 km), respectively, with the left-bottom corner of a square as the origin point \((x, y) = (0 \text{ km}, 0 \text{ km})\). Figs. 3a and b show the vertical profiles of the \(P\) and \(S\)-velocity structures for cases (a) and (b), respectively. For the source, we use a point single force with the Ricker-wavelet as the source time function:

\[
 f_\alpha(t, \vec{x}) = g_\alpha \left( \frac{2\pi^2 t^2}{t_d^2} - 1 \right) \exp \left( -\frac{\pi^2 t^2}{t_d^2} \right) \delta(\vec{x} - \vec{x}_s), \tag{5.3}
\]

where \(\alpha\) represents \(x\), and \(y\)-axes, \(\vec{x}_s\) is the location of the source, \(g_\alpha\) are constants, and \(t_d\) is the central period. Here, we use \((g_x, g_y) = (1 \text{ N}, 1 \text{ N})\) and \(t_d = 4 \text{ s}\). Firstly, we consider case (a): a homogeneous model with \(\rho = 5 \text{ g/cm}^3\), \(V_P = 10 \text{ km/s}\), and \(V_S = 5 \text{ km/s}\), which are exactly same as those used for the dispersion analysis shown above.

For discretization, we use the Cartesian grid with the length of an element along the \(x\) and \(y\)-axes given by \(\Delta x = \Delta y = h\), where cases of several values of \(h\) are considered. We set the time interval as \(\Delta t = 0.05(h/n)/V_P = 0.005h/n\). The value of \(\Delta t\) used in this section may be rather strict compared with that used in actual applications of the SEM \([1, 5]\), in order to remove out the error due to the temporal discretization, on which we do not focus in this study. We use our modified operators for the numerical spatial integration for each element except for the elements in contact with the bottom and left boundaries, along which we cannot implement the modified operator of Eq. (3.33) by the definition. Thus, we use the ordinary SEM operators only for these elements. For the numerical temporal integration, we use the second-order finite-difference operator. Note that although the mass matrix based on our method is, unfortunately, no longer diagonal, we can avoid computing the inverse mass matrix by using a predictor-corrector scheme for a non-diagonal mass matrix \([25]\) (see Appendix C for detailed description). The temporal integration is considered for the time from \(t_0 = -8 \text{ s}\) to \(t_1 = 292 \text{ s}\). For comparison, we also make the same computation using the ordinary SEM operators.

Fig. 4a shows the error of the waveforms at the receiver, computed by using our method and the SEM of several orders. The errors are plotted as functions of the average number of grid points per wavelength \(G_d\). We define \(G_d\) as follows:

\[
 G_d = \frac{\lambda_d}{h/n} = \frac{nV_s t_d}{h}, \tag{5.4}
\]

where \(\lambda_d\) denotes the length of the \(S\)-wavelet excited by the source of Eq. (5.3), and we assume that \(\lambda_d\) is simply defined as the wavelength of the harmonic \(S\)-wave with the central period \(t_d = 4 \text{ s}\). We evaluate the error of a waveform as follows:

\[
 \text{Waveform Error} = \sqrt{\int_{t_0}^{t_1} |\vec{u}^{\text{num}}(t) - \vec{u}^{\text{exact}}(t)|^2 \, dt / \int_{t_0}^{t_1} |\vec{u}^{\text{exact}}(t)|^2 \, dt} \times 100 \%, \tag{5.5}
\]

where \(\vec{u}^{\text{num}}\) is the displacement computed numerically, and \(\vec{u}^{\text{exact}}\) is the exact solution that is computed by using the SEM with higher-order elements and an extremely fine grid \((n = 5 \text{ and } G_d = 40)\).

We see from Fig. 4a that our method has higher accuracy than the SEM of the same order, and is roughly comparable to the SEM of one order higher, thanks to the dispersionless nature of our method. More precisely, the accuracy of our method of order \(n \leq 2\) seems to become slightly inferior to the SEM of one order higher with larger value of \(G_d\). This may be due to the errors caused from boundary elements or the force term, on which we do not focus in our modification. Both for the methods of order \(n \geq 3\), the accuracy seems to be somewhat plateauing when the error is smaller than 1 %. In those cases, the error due to the numerical temporal integration is no longer negligible despite the small time interval. Fig. 5 shows a comparison of the error of waveforms computed by using our method and the SEM. Both for the methods, we use \(n = 2\) and \(G_d = 16\). In this case, the errors of our method and the SEM are 2.4 and 19.1 %, respectively. Then, the error of our method is roughly 7 times smaller than that of the SEM. The CPU-time required for computation using our method is roughly 1.4-1.7 times larger than that for the SEM of the same order, regardless of the number and order of elements.
Next, we consider case (b): a vertically heterogeneous model with $P$ and $S$-velocity structure shown in Fig. 3b. The velocity structures are fluctuated as trigonometric functions with the wavelength 200 km and with the amplitude 20% from the standard velocities $V_P = 10\text{km/s}$ and $V_S = 5\text{km/s}$, respectively. The density $\rho$ and the other settings including the value of $\Delta t$ and the definition of $G_d$ are same as case (a). Fig. 4b shows the error of the waveforms computed by using our method and the SEM of several orders. Although the accuracy of our method seems to be slightly degraded, we see similar trends in case (a). Since we use the same codes as case (a), so is the CPU-time.
Fig. 1: Numerical dispersion versus the average number of grid points per wavelength $G$. $\theta$ denotes the angle between the wavenumber vector $\vec{k}$ and the positive $x$-axis. Left, center, and right panels show for $\theta = 0^\circ$, $30^\circ$, and $45^\circ$, respectively, and top and bottom panels for $P$ and $S$-waves. The solid and dash lines correspond to our method and the SEM, respectively. For each case, colors red, blue, green, and orange correspond to orders $n = 1$, $2$, $3$, and $4$, respectively, and cyan corresponds to the SEM of order $n = 5$. 
Fig. 2: A schematic illustration of the 2-D models used in the waveform computations of Section 5. The star and triangle indicate the locations of source and receiver points, respectively.

Fig. 3: The vertical (the y-directional) dependences of the velocity structures used in the waveform computations of Section 5. The dash and solid lines show the P and S-wave velocities, respectively. (a) The homogeneous case. (b) The vertically heterogeneous case.
Fig. 4: The error of computed waveforms versus the average number of grid points per wavelength $G_d$. The solid and dash lines correspond to our method and the SEM, respectively. For each case, colors red, blue, green, and orange correspond to $n = 1, 2, 3,$ and $4$, respectively, and cyan corresponds to the SEM of $n = 5$. (a) The homogeneous case. (b) The vertically heterogeneous case.

Fig. 5: Waveform errors. (top panel) The first trace shows the $x$-component of the exact waveform used for case (a). The second trace shows the $x$-component of the residual of a waveform computed by our method minus the exact one, and the third trace shows the residual for the SEM (both of the traces are amplified by 5 times). We show for $n = 2$ and $G_d = 16$. (bottom panel) The same as the top panel, except for the $y$-component.
6. Conclusions and future outlook

We derived modified numerical integration operators for the SEM for simulation of elastic wave propagation. The modification was constructed for the respective operator errors to be canceled out, which yields the superior accuracy compared to the original SEM of the same order. We also showed numerical dispersion analysis and examples of computation of waveforms using our operators, which followed our theoretical results. While the optimally blending operator (3.29) itself has been previous presented by [20] with a rather strict approach, we derived it on the basis of a perturbation error analysis [27], which simplifies the derivation. Furthermore, we extended this approach to elastic wave computation.

This paper did not consider anelastic media. We would be obliged to make some changes to the elastic wave equation with such as the memory variable formulation for anelastic media [29]. However, our operators would still improve the accuracy, since the numerical dispersion would be a primary factor in the numerical error. This extension yet should be an important subject for future work.

In the definition of our operators, we assumed the Cartesian grid. However, a use of deformed grids can more flexibly meet configurations of surface and internal boundaries. Nevertheless, as shown by [30], we can consider a mapping from a model structure with irregular boundaries onto a reference model with flat boundaries using a coordinate transformation before the spatial discretization. we will then be able to treat irregular boundaries with a slight modification.

Acknowledgement

This research was partly supported by grants from the Ministry of Science and Technology of Taiwan (MOST 106-2811-M-001-158). N. F. is partly supported by GPX consortium of Institut de Physique du Globe de Paris, École des Mines de Paris, Schlumberger, CGG, TOTAL, and Agence Nationale de la Recherche of France (ANR).

Appendix A. Basic formulas

In the definition of the numerical integration operators and their error analysis in Section 3, we often use the following lemma:

\[ \int_{-1}^{1} P_n(x) x^l \, dx = 0 \quad \text{if } l < n, \quad (A.1) \]

where \( P_n \) is the Legendre polynomial of the \( n \)-th-order, and \( l \) is a non-negative integer. It is clearly seen from the well-known orthogonality relation:

\[ \int_{-1}^{1} P_{n'}(x) P_n(x) \, dx = \frac{2}{2n+1} \delta_{n'n}, \quad (A.2) \]

where \( n' \) is a natural number. We immediately have Eq. (A.1), because \( x^l \) \((l < n)\) can be written as a linear combination of the Legendre polynomials of order below \( n \), and those are orthogonal to \( P_n \).

Noting that \( P_n \) is a polynomial of degree \( n \), it can be written as

\[ P_n(x) = r_n x^n + o(x^{n-1}), \quad (A.3) \]

or, conversely, we have

\[ x^n = r_n^{-1} P_n(x) + o(x^{n-1}), \quad (A.4) \]

where \( r_n \) is the coefficient of the term of degree \( n \), and \( o(x^l) \) represents terms of degree \( l \) or below. Note that \( o(x^l) \) is not to be confused with \( O(x^l) \), where \( O(x^l) \) represents terms of degree \( l \) or above. From Eqs. (A.2) and (A.4), we have

\[ \int_{-1}^{1} P_n(x) x^n \, dx = \frac{2}{2n+1} r_n^{-1}. \quad (A.5) \]
We consider the $n$-th-order Gauss-Lobatto-Legendre (GLL) quadrature rule, by which an integral is exactly computed when the integrand is a polynomial of degree $(2n - 1)$ or below. Then, noting that the degree of the integrand of Eq. (A.1) is $(2n - 1)$ or below, Eq. (A.1) can be rewritten as follows:

$$
\sum_{i=0}^{n} q_i P_n(x_i)x_i^l = 0 \quad \text{if} \ l < n,
$$

(A.6)

where $x_i$ and $q_i$ ($i = 0, \ldots, n$) are the GLL quadrature nodes and weights, respectively.

The GLL nodes (3.13) are the zeros of the following polynomial of degree $(n + 1)$:

$$
U(x) \equiv (x^2 - 1) P'_n(x).
$$

(A.7)

Then, by the definition of $x_i$, $U$ satisfies

$$
U(x) \propto \prod_{i=0}^{n} (x - x_i).
$$

(A.8)

The GLL weights are given by

$$
q_i = \int_{-1}^{1} L_i(x)dx = \frac{2}{n(n+1)[P_n(x_i)]^2},
$$

(A.9)

where $L_i$ are the Lagrange interpolating polynomials (3.14).

An arbitrary polynomial of degree $n$ or below can be exactly expressed in terms of a polynomial basis of degree $n$. Then, the constant 1 can be written by a linear combination of $L_i$ ($i = 0, \ldots, n$) as follows:

$$
1 = \sum_{i=0}^{n} L_i(x).
$$

(A.10)

Taking the differentiation of Eq. (A.10), we have

$$
\sum_{i=0}^{n} L'_i(x) = 0.
$$

(A.11)

For the same reason, the $(n + 1)$-th-order Lagrange interpolating polynomials (3.31) satisfy

$$
\sum_{i=-1}^{n} X'_i(x) = 0.
$$

(A.12)

In addition, we list some notable formulas. The following formulas are well-known, or can be obtained by using well-known formulas with some algebra, and thus here we omit their derivations:

$$
\int_{-1}^{1} 1dx = \sum_{i=0}^{n} q_i = 2
$$

(A.13)

$$
U(x) = (x^2 - 1)P'_n(x) = (n + 1) [P_{n+1}(x) - xP_n(x)]
$$

$$
U'(x) = [(x^2 - 1)P'_n(x)]' = n(n + 1)P_n(x)
$$

(A.14)

$$
L_i(x) = \delta_{ij}
$$

(A.15)

$$
L_i(x) = \frac{1}{U'(x_i)} \frac{U(x)}{x - x_i} = \frac{1}{n + 1} P_n(x) + o(x^{n-1})
$$

(A.16)
\[
\frac{L_i(x) - L_i(x_j)}{x - x_j} = \frac{n r_n}{U'(x_i)} x^{n-1} + o(x^{n-2}) \quad (A.18)
\]

\[
L_i'(x) = \frac{P_n(x) - L_i(x)}{x-x_i} \quad (A.19)
\]

\[
L_i'(x_j) = \frac{P_n'(x_i)}{2P_n(x_i)} \delta_{ij} + \frac{1 - \delta_{ij}}{P_n(x_i)} \frac{1}{x-x_i} \quad (A.20)
\]

\[
X_i(x_j) = \delta_{ij} \quad (A.21)
\]

\[
X_i(x) = \begin{cases} 
L_i(x) + \frac{1}{U'(x_i)} \frac{U(x)}{x-x_i} & \text{if } i \neq -1 \\
L_i(x) + \frac{1}{U'(x_{i-1})} \frac{U(x)}{x-x_i} & \text{if } i = -1 
\end{cases} \quad (A.22)
\]

\[
X_i'(x) = \begin{cases} 
L_i'(x) + \frac{P_n(x)}{(x_i - x_{i-1})P_n(x_i)} & \text{if } i \neq -1 \\
\frac{n(n+1)P_n(x)}{(x^2-1)P_n'(x-1)} & \text{if } i = -1,
\end{cases} \quad (A.23)
\]

where \(i, j = 0, \ldots, n\), except for Eqs. \((A.21)-(A.23)\); in those cases, we consider \(i, j = -1, 0, \ldots, n\).

Finally, we note some integration results. Using the above equations with some algebra, we have

\[
\int_{-1}^{1} L_i(x)L_j(x)dx = \frac{1}{U'(x_i)} \int_{-1}^{1} \frac{U(x)}{x-x_i} L_j(x)dx
\]

\[
= \frac{L_j(x_i)}{U'(x_i)} \int_{-1}^{1} \frac{U(x)}{x-x_i} dx + \frac{1}{U'(x_i)} \int_{-1}^{1} \frac{U(x)}{x-x_i} \frac{L_j(x) - L_i(x_i)}{x-x_i} dx
\]

\[
= \frac{L_j(x_i)}{U'(x_i)} \int_{-1}^{1} L_i(x)dx + \frac{n(n+1)r_n}{U'(x_i)U'(x_j)} \int_{-1}^{1} \left[ P_{n+1}(x) - xP_n(x) \right] \left[ x^{n-1} + o(x^{n-2}) \right] dx
\]

\[
= \delta_{ij}q_i - \frac{n(n+1)}{2(2n+1)} q_i P_n(x_i) q_j P_n(x_j). \quad (A.24)
\]

The result is used for defining \(A^{FE\text{M}}\) and \(A^{opt}\) of Eqs. \((3.27)\) and \((3.29)\). For \(C^{opt}\) of Eq. \((3.33)\), we use the following integration results:

\[
\int_{-1}^{1} L_i(x)P_n(x)dx = \frac{1}{(n+1)P_n(x_i)} \int_{-1}^{1} \left[ P_n(x) + o(x^{n-1}) \right] P_n(x)dx
\]

\[
= \frac{n}{2n+1} q_i P_n(x_i). \quad (A.25)
\]

\[
\int_{-1}^{1} X_{i>-1}'(x)L_j(x)dx = \int_{-1}^{1} L_i'(x)L_j(x)dx + \frac{n^2(n+1)}{2(2n+1)} \frac{q_i P_n(x_i) q_j P_n(x_j)}{x_i - x_{i-1}} \quad (A.26)
\]

\[
\int_{-1}^{1} X_{i-1}'(x)L_j(x)dx = \frac{n^2(n+1)}{2n+1} \frac{q_i P_n(x_i)}{(x_{i-1} - 1)P_n'(x_{i-1})}. \quad (A.27)
\]

Appendix B. Harmonic responses of numerical integration operators

Herein, we derive Eqs. \((3.22)-(3.24), (3.28), and (3.34)-(3.36)\). For these purposes, we evaluate the quadratic form with \((\phi, \psi) = (p^*_h, p_h)\) for each integration operator. Then, we can immediately obtain the response errors by comparing them with the exact values given by Eqs. \((3.19)-(3.21)\). \(A^{SEM}(p^*_h, p_h)\) is
immediately obtained as follows:

\[ A^{SEM}(p_h^*, p_h) = \sum_{i=0}^{n} q_i = 2, \]  

(B.1)

where we use Eq. (A.13). \( A^{SEM}(p_h^*, p_h) \) is evaluated as follows:

\[
A^{SEM}(p_h^*, p_h) = 2 - \frac{n(n+1)}{2(2n+1)} \left| \sum_{i=0}^{n} q_i p_n(x_i) e^{ihx_i} \right|^2 \\
= 2 - \frac{n(n+1)}{2(2n+1)} \left| \sum_{i=0}^{n} q_i p_n(x_i) \sum_{l=0}^{\infty} \frac{(ihx_i)^l}{l!} \right|^2 \\
= 2 - \frac{n(n+1)\hat{h}^{2n}}{2(2n+1)(n!)^2} \left[ \sum_{i=0}^{n} q_i p_n(x_i)x_i^n \right]^2 + O(\hat{h}^{2n+2}) \\
= 2 + 2(n+1)E_n \hat{h}^{2n} + O(\hat{h}^{2n+2}),
\]

(B.2)

where \( E_n \) is given by Eq. (3.25), and we use Eq. (A.16) for the derivation of the third line. Then, using the first line of Eq. (3.29), and Eqs. (B.1) and (B.2), we immediately obtain

\[ A^{opt}(p_h^*, p_h) = 2 + 2E_n \hat{h}^{2n} + O(\hat{h}^{2n+2}). \]

(B.3)

In order to evaluate \( B^{SEM}(p_h^*, p_h) \), we make the following algebra:

\[
S_j = \sum_{i=0}^{n} e^{ihx_i} L_i'(x_j) \\
= e^{ihx_j} \sum_{i=0}^{n} e^{ih(x_i-x_j)} - 1 \left[ e^{ih(x_i-x_j)} - 1 \right] L_i'(x_j) \\
= e^{ihx_j} \sum_{i=0, i \neq j}^{n} e^{ih(x_i-x_j)} - 1 \left[ e^{ih(x_i-x_j)} - 1 \right] L_i'(x_j) \\
= -e^{ihx_j} P_n(x_j) \sum_{i=0, i \neq j}^{n} \frac{1}{P_n(x_i)} \frac{e^{ih(x_i-x_j)} - 1}{x_i - x_j} \\
= -e^{ihx_j} P_n(x_j) \sum_{i=0, i \neq j}^{n} \frac{1}{P_n(x_i)} \sum_{l=1}^{\infty} \frac{(ih)^l(x_i-x_j)^{l-1}}{l!} \\
= -e^{ihx_j} P_n(x_j) \left[ 1 - \delta_{ij} \right] \sum_{i=0}^{n} \frac{(ih)^l(x_i-x_j)^{l-1}}{l!} \\
= \left[ i\hat{h} - \frac{n(n+1)}{2} P_n(x_j) R_j \right] e^{ihx_j},
\]

(B.4)

where \( R_j \) in the last line is

\[ R_j = \sum_{i=0}^{n} q_i P_n(x_i) \sum_{l=1}^{\infty} \frac{(ih)^l(x_i-x_j)^{l-1}}{l!}. \]

(B.5)

Note that we use Eq. (A.11) for the derivation of the second line of Eq. (B.4), and Eq. (A.20) for the fourth line. Further, we evaluate the following values:

\[ I = \sum_{j=0}^{n} |R_j|^2 \]
\[ J \equiv \sum_{j=0}^{n} q_{j} P_{n}(x_{j})(R_{j} - R_{j}^{*}) \]
\[ J = \sum_{i,j=0}^{\infty} q_{j} P_{n}(x_{i})q_{i} P_{n}(x_{i}) \sum_{l=0}^{\infty} \frac{2(i\hbar)^{2l+1}(x_{i} - x_{j})^{2l}}{(2l + 1)!} \]
\[ J = i\hbar^{2n+1} \frac{2(2n)^{n} \left( \sum_{i=0}^{n} q_{i} P_{n}(x_{i})x_{i}^{n} \right)^{2}}{(2n + 1)!} + O(\hbar^{2n+3}), \quad (B.7) \]

where we use Eq. (A.6) and \( (\begin{pmatrix} n \\ 2 \end{pmatrix} ) \) denotes the binomial coefficient of the \( x_{i}^{n}x_{j}^{n} \) term in the expansion of \( (x_{i} - x_{j})^{2n} \). Finally, we obtain

\[ B_{SEM}^{*}(p^{*}_{h}, p_{h}) = \sum_{j=0}^{n} q_{j} |S_{j}|^{2} \]
\[ = \sum_{j=0}^{n} q_{j} \left| i\hbar - \frac{n(n + 1)}{2} P_{n}(x_{j})R_{j} \right|^{2} \]
\[ = 2\hbar^{2} + \frac{n(n + 1)}{2} I + i\hbar \frac{n(n + 1)}{2} J \]
\[ = 2\hbar^{2} + 2\varepsilon_{n} \hbar^{2n+2} + O(\hbar^{2n+4}). \quad (B.8) \]

\( C_{SEM}^{*}(p^{*}_{h}, p_{h}) \) is evaluated as follows:

\[ C_{SEM}^{*}(p^{*}_{h}, p_{h}) = \sum_{j=0}^{n} q_{j} e^{i\hbar x_{j}x_{j}^{*}} \]
\[ = \sum_{j=0}^{n} q_{j} \left[ -i\hbar - \frac{n(n + 1)}{2} P_{n}(x_{j})R_{j}^{*} \right] \]
\[ = -2i\hbar - \frac{n(n + 1)}{2} \sum_{i,j=0}^{n} q_{j} P_{n}(x_{j})q_{i} P_{n}(x_{i}) \sum_{l=1}^{\infty} \frac{(-i\hbar)^{l}(x_{i} - x_{j})^{l-1}}{l!} \]
\[ = -2i\hbar - \frac{n(n + 1)}{2} \sum_{i,j=0}^{n} q_{j} P_{n}(x_{j})q_{i} P_{n}(x_{i}) \left( -i\hbar \right)^{2n+1} \left( \begin{pmatrix} n \\ 2 \end{pmatrix} \right)^{n} \left( x_{i}^{n}(-x_{j})^{n} \right) \left( 2n + 1 \right)! \]
\[ = -2i\hbar - i\hbar^{2n+1} \frac{n(n + 1) \left( \begin{pmatrix} n \\ 2 \end{pmatrix} \right)^{n}}{2(2n + 1)!} \left( \sum_{i=0}^{n} q_{i} P_{n}(x_{i})x_{i}^{n} \right)^{2} + O(\hbar^{2n+2}) \]
\[ = -2i\hbar - 2i(n + 1)\varepsilon_{n} \hbar^{2n+1} + O(\hbar^{2n+2}), \quad (B.9) \]

where we use Eq. (A.6) for the derivation of the fourth line.

To evaluate \( C_{opt}^{*}(p^{*}_{h}, p_{h}) \), we make the following algebra:

\[ T(x) \equiv \sum_{i=-1}^{n} e^{i\hbar x_{i}X_{i}^{*}(x)} \]
or a non-zero pure imaginary term at the (2

the last line of Eq. (B.12), we see after algebra that it is zero or a real number. Hence, Eq. (3.36) has zero

in the second line. Note that although we here omit the evaluation of the coefficient of the \( \hat{x} \), where we use Eq. (A.6) for the derivation of the fourth line, and Eq. (A.25) for calculation of the integral

where we use Eqs. (A.12) and (A.23) for the derivation of the second and fourth lines of Eq. (B.10), respectively, and Eq. (A.6) for the derivation of the third line of Eq. (B.11). Finally, \( C_{opt}^{pt}(p_h^*, p_h) \) is evaluated as follows:

\[
C_{opt}^{pt}(p_h^*, p_h) = \int_{-1}^{1} [T(x)]^n \sum_{j=0}^{n} e^{i \hat{h} x_j} L_j(x) dx
\]

\[
= \sum_{i,j=0}^{n} e^{i \hat{h} (x_j - x_i)} \int_{-1}^{1} L_i'(x) L_j(x) dx + H^* \sum_{j=0}^{n} e^{i \hat{h} (x_j - x_i)} \int_{-1}^{1} L_j(x) P_n(x) dx
\]

\[
= C_{SEM}^{pt}(p_h^*, p_h) + \frac{n H^*}{2 n + 1} \sum_{j=0}^{n} q_i P_n(x_j) e^{i \hat{h} (x_j - x_i)}
\]

\[
= C_{SEM}^{pt}(p_h^*, p_h) + (i \hat{h})^n \frac{n H^*}{(2 n + 1) n} \sum_{j=0}^{n} q_i P_n(x_j) x_j^n + O(\hat{h}^{n+1}) H^*
\]

\[
= C_{SEM}^{pt}(p_h^*, p_h) + 2 i m \mathcal{E}_n \hat{h}^{2 n + 1} + O(\hat{h}^{2 n + 2})
\]

\[
= -2 i \hat{h} - 2 i m \mathcal{E}_n \hat{h}^{2 n + 1} + O(\hat{h}^{2 n + 2}),
\]

where we use Eq. (A.6) for the derivation of the fourth line, and Eq. (A.25) for calculation of the integral in the second line. Note that although we here omit the evaluation of the coefficient of the \( \hat{h}^{2 n + 2} \) term in the last line of Eq. (B.12), we see after algebra that it is zero or a real number. Hence, Eq. (3.36) has zero or a non-zero pure imaginary term at the \((2 n + 1)\)-th-order.

Appendix C. Predictor-corrector scheme for explicit time-marching

Numerical integration operator \( A_{opt}^{pt} \) of Eq. (3.29) is no longer diagonal. Then, supposing that the mass matrix is defined on the basis of \( A_{opt}^{pt} \), as shown in Eq. (4.15) or (4.22), it will not be consequently diagonal. In that case, the inverse mass matrix would not be easily obtained. However, we can avoid computing the inverse mass matrix by applying a predictor-corrector time-marching scheme for a non-diagonal mass matrix [28]. Here, we reformulate the scheme of [28] to be applicable to our method.

\[\begin{align*}
&= e^{i \hat{h} x_{i-1}} \sum_{i=1}^{n} \left[ e^{i \hat{h} (x_i - x_{i-1})} - 1 \right] X'_i(x) \\
&= e^{i \hat{h} x_{i-1}} \sum_{i=0}^{n} \left[ e^{i \hat{h} (x_i - x_{i-1})} - 1 \right] X'_i(x) \\
&= \sum_{i=0}^{n} e^{i \hat{h} x_i} L'_i(x) + e^{i \hat{h} x_{i-1}} \sum_{i=0}^{n} P_n(x) e^{i \hat{h} (x_i - x_{i-1})} - 1 \\
&= \sum_{i=0}^{n} e^{i \hat{h} x_i} L'_i(x) + e^{i \hat{h} x_{i-1}} H P_n(x),
\end{align*}\]

where \( H \) in the last line is

\[
H = \sum_{i=0}^{n} \frac{1}{P_n(x_i)} e^{i \hat{h} (x_i - x_{i-1})} - 1 \\
= \frac{n(n+1)}{2} \sum_{i=0}^{n} q_i P_n(x_i) \sum_{l=1}^{\infty} \frac{(i \hat{h})^l (x_i - x_{i-1})^{l-1}}{l!} \\
= (i \hat{h})^n + \frac{n}{2 n + 1} \sum_{i=0}^{n} q_i P_n(x_i) x_i^n + O(\hat{h}^{n+1}).
\]

Note that we use Eqs. (A.12) and (A.23) for the derivation of the second and fourth lines of Eq. (B.10), respectively, and Eq. (A.6) for the derivation of the third line of Eq. (B.11).
Supposing that the mass and stiffness matrices are constructed based on our modified operators, the time-domain discrete form of the wave equation can be written as follows:

\[ M_{opt} \dot{a}_t = -K_{opt} u_t + F, \quad (C.1) \]

where \( M_{opt} \) and \( K_{opt} \) are the mass and stiffness matrices, \( u_t \) and \( a_t \) are the discretized displacement and acceleration at the time \( t \), respectively, and \( F \) is the force term. Here, we suppose that the acceleration \( a_t \) is approximated by the second-order finite-difference operator as follows:

\[ a_t = \frac{u_{t+\Delta t} - 2u_t + u_{t-\Delta t}}{\Delta t^2}, \quad (C.2) \]

where \( \Delta t \) is the time interval, and \( u_{t+\Delta t} \) and \( u_{t-\Delta t} \) are the discretized displacements at the time \( t + \Delta t \) and \( t - \Delta t \), respectively. Note that \( u_t \) and \( u_{t-\Delta t} \) are the variables already known, whereas the elements of \( u_{t+\Delta t} \) are the unknown variables to be solved from Eqs. (C.1) and (C.2).

We rewrite \( A_{opt} \) as follows:

\[ A_{opt} = A_{SEM} + \epsilon A_{corr}, \quad (C.3) \]

where the first and second terms of the right-hand side respectively correspond to those of the second line of Eq. (3.29). Note that the first term \( A_{SEM} \) is equal to the diagonal operator of the SEM, whereas \( \epsilon A_{corr} \) is a non-diagonal operator which will have small contribution to the numerical computation. Given that mass matrix is expressed as the three-fold tensor product of \( A_{opt} \) with itself for \( x, y, z \)-axes (or the two-fold tensor product for the 2-D case as shown in Eq. 4.15 or 4.22), the mass matrix can be expanded as a cubic function of \( \epsilon \) (or a quadratic function for the 2-D case). For the 3-D case, \( M_{opt} \) is expanded as follows:

\[ M_{opt} = M_{SEM} + \epsilon M_{corr1} + \epsilon^2 M_{corr2} + \epsilon^3 M_{corr3}, \quad (C.4) \]

where \( M_{SEM} \) is the diagonal mass matrix given as the three-fold tensor product of \( A_{SEM} \) with itself for \( x, y, z \)-axes, and \( \epsilon M_{corr1}, \epsilon^2 M_{corr2}, \) and \( \epsilon^3 M_{corr3} \) are matrices which contain a single \( \epsilon A_{corr} \), and its two and three-fold tensor products, respectively. If we replace \( M_{opt} \) of Eq. (C.1) by \( M_{SEM} \), we obtain the following equation:

\[ M_{SEM} \ddot{a}_t = -K_{opt} u_t + F, \quad (C.5) \]

with a vector \( \ddot{a}_t \).

Now we assume that the contribution from \( \epsilon A_{corr} \) is sufficiently small so that the last two terms of the right-hand side of Eq. (C.4) will be negligible as follows:

\[ M_{opt} \approx M_{SEM} + \epsilon M_{corr1}. \quad (C.6) \]

Similarly, we assume that \( a_t \) of Eq. (C.1) is well-approximated as the first-order perturbation from \( \ddot{a}_t \) as follows:

\[ a_t \approx \ddot{a}_t + \epsilon a_{corr}, \quad (C.7) \]

where \( \epsilon a_{corr} \) is a small correction term. Substituting Eqs. (C.6) and (C.7) into Eq. (C.1), and taking the first-order terms of \( \epsilon \), we have

\[ M_{SEM} \epsilon a_{corr} = -\epsilon M_{corr1} \ddot{a}_t. \quad (C.8) \]

Since \( M_{SEM} \) is diagonal, \( \epsilon a_{corr} \) can be immediately obtained from the equation. We use Eqs. (C.5), (C.7), and (C.8), instead of Eq. (C.1), and then we obtain \( u_{t+\Delta t} \) for the next time step from Eq. (C.2). Note that the above scheme may be also applicable to any other numerical temporal finite-difference operators, rather than Eq. (C.2).
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