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Stable modeling of free boundaries in the finite-difference time-domain method using staggered grids with collocated grid points of velocities

SGCV を用いた FDTD 法における自由境界の安定な取り扱い

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1. Introduction

The finite-difference time-domain (FDTD) method has simple schemes for approximating space and time derivatives of fields with discretized field values at grid points. For analysis of elastic waves propagating in solids by the FDTD method, we first choose the grids from standard staggered grids (SSG),[1)] Lebedev grids,[2)] rotated staggered grids,[3)] or staggered grids with the collocated grid points of velocities (SGCV).[4, 5)] The SGCV was developed for simple imposing of boundary conditions: free boundaries, symmetry condition, and asymmetry condition. Although FDTD analyses of isotropic and quartz Lamé resonators demonstrated the validity and usefulness of the SGCVs, the stability of SGCV models with free boundaries should be improved for long time simulation such as $2^{20} \cong 10^{6.02}$ time steps.

In this paper, we presented two stable SGCV models of free boundaries in two dimensions. These models impose stress-free condition on the velocity fields in the SGCV half grids which are adjacent to the free boundary with bilinear polynomial interpolations. The stability and validity of the models were demonstrated by computing resonant frequencies of an isotropic Lamé resonator in the finite-difference frequency-domain (FDFD) method.

2. Stable SGCV models of free boundaries

Figure 1 shows three SGCV models of free boundaries in two dimensions ($\partial/\partial z = 0$). Here, $\boldsymbol{p}_{\mathrm{T}}$ and $\boldsymbol{p}_i$ ($i = 1,2,3,4$) are position vectors of the grid points $\mathrm{P_T}$ and $\mathrm{P_i}$ of stress components and velocity components, respectively. In the SGCV grid with the second order accuracy in spatial approximation, a velocity vector $\boldsymbol{v}(\boldsymbol{r})$ at a point with the position vector $\boldsymbol{r} = \hat{x}x + \hat{y}y$ can be expressed as follows:

$$\boldsymbol{v}(\boldsymbol{r}) = \boldsymbol{C}_{00} + (x - x_0)\boldsymbol{C}_{10} + (y - y_0)\boldsymbol{C}_{01} + (x - x_0)(y - y_0)\boldsymbol{C}_{11}. \qquad (1)$$

Here, the vector coefficients $\boldsymbol{C}_{lm}(l, m = 0,1)$ can be determined from the values at the four vertices of the SGCV grid with a reference point $(x_0,\ y_0)$.

We consider computation of the values $T_{xy}(\boldsymbol{p}_{\mathrm{T}})$ and $T_{yy}(\boldsymbol{p}_{\mathrm{T}})$ with the SGCV grids as shown in figure 1. For computing the strain components $S_{xx}(\boldsymbol{p}_{\mathrm{T}})$ and $S_{yx}(\boldsymbol{p}_{\mathrm{T}}) = S_{xy}(\boldsymbol{p}_{\mathrm{T}})$,

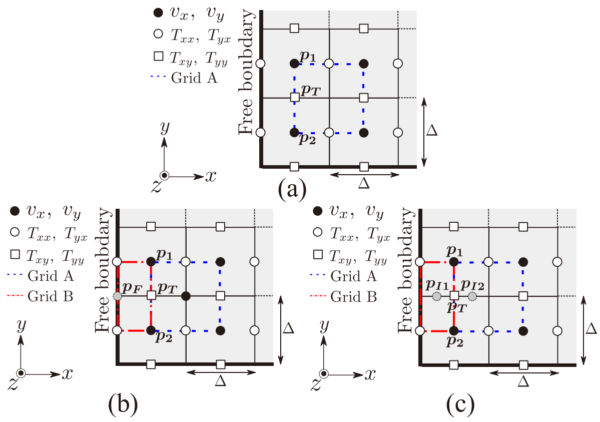

Fig. 1 SGCV models of free boundaries: (a) conventional SGCV model (CSGCVM), (b) stable SGCV model using a velocity in the free boundary (SGCVMVF), (c) stable SGCV model using velocity derivatives at the centers of adjacent half grids (SGCVMVD).

the conventional SGCV model (CSGCVM) shown in figure 1 (a) uses the values of derivatives $\partial\boldsymbol{v}(\boldsymbol{r})/\partial x|_{\boldsymbol{r}=\boldsymbol{p}_T}$ by differentiating (1) for the grid A with sides Δ. Here, we do not use the stress-free boundary conditions, $T_{xx} = 0$ and $T_{yx} = 0$. In stable SGCV models of free boundaries, imposing the stress-free conditions on (1) for the half grid B being $\Delta/2 \times \Delta$ in area shown in Fig. 1 (b) and (c), and substituting $\boldsymbol{v}(\boldsymbol{r})$ in (1) with the values $\boldsymbol{v}(\boldsymbol{p}_1)$ and $\boldsymbol{v}(\boldsymbol{p}_2)$, we can determine $\boldsymbol{C}_{lm}$ from $\boldsymbol{v}(\boldsymbol{p}_1)$ and $\boldsymbol{v}(\boldsymbol{p}_2)$, and compute $\boldsymbol{v}(\boldsymbol{p}_{\mathrm{F}})$ from (1) for SGCVMVF and $\partial\boldsymbol{v}(\boldsymbol{r})/\partial x|_{\boldsymbol{r}=\boldsymbol{p}_{\mathrm{I1}}}$ by differentiating (1) for SGCVMVD. Using (1) for the grid A, we have the value of $\boldsymbol{v}(\boldsymbol{p}_{\mathrm{c}})$ for SGCVMVF or $\partial\boldsymbol{v}(\boldsymbol{r})/\partial x|_{\boldsymbol{r}=\boldsymbol{p}_{\mathrm{I2}}}$ for SGCVMVD. Hence, we can determine required values as follows: $\partial\boldsymbol{v}(\boldsymbol{r})/\partial x|_{\boldsymbol{r}=\boldsymbol{p}_T} \approx (\boldsymbol{v}(\boldsymbol{p}_{\mathrm{F}}) - \boldsymbol{v}(\boldsymbol{p}_{\mathrm{c}}))/\Delta$ for SGCVMVF and $\partial\boldsymbol{v}(\boldsymbol{r})/\partial x|_{\boldsymbol{r}=\boldsymbol{p}_{\mathrm{T}}} \approx (\partial\boldsymbol{v}(\boldsymbol{r})/\partial x|_{\boldsymbol{r}=\boldsymbol{p}_{\mathrm{I1}}} + \partial\boldsymbol{v}(\boldsymbol{r})/\partial x|_{\boldsymbol{r}=\boldsymbol{p}_{\mathrm{I2}}})/2$ for SGCVMVD.

3. Stability analysis of FDTD models

We used von Neumann stability analysis of FDTD models of a two-dimensional Lamé-mode resonator on an isotropic plate: applying central difference approximation with the second order accuracy to the spatial derivatives in Newton's equation of motion and the strain-displacement relation with the elastic constitutive equation, we have

$$\frac{\partial f^{(n)}}{\partial t} = R\,A\,\frac{f^{(n)}}{\Delta_t} \qquad (2)$$

where $R = V_p \Delta_t/\Delta$ is the Courant number, $\{f^{(n)}\}^{\mathrm{T}} = [\{v^{(n)}\}\{T^{(n)}\}]$, t, A, Δ_t, and V_p are time, the normalized matrix of finite difference spatial operator, a time interval, and the velocity of the longitudinal bulk wave in the isotropic solid. Here, the superscript (n) and T denote the values at the time $t = n\Delta_t$ and transpose of the column vector, and $\{v^{(n)}\}$ and $\{T^{(n)}\}$ are two column vectors composed of the velocity and the stress components at all FDTD grid points, respectively. Assuming that the elastic fields are time-harmonic fields with angular frequency ω, we have $f^{(n)} = f_\omega e^{j\omega n\Delta_t}$ and we can derive an eigenvalue problem from (2) as follows:

$$\left(\frac{j\omega\Delta_t}{R}\right) f_\omega = A f_\omega \qquad (3)$$

where $(j\omega\Delta_t/R)$ and f_ω are the eigenvalue and the eigenvector of the matrix A.

Next, using the second order approximation of the time derivative in (2), $\partial f^{(n)}/\partial t \approx (f^{(n+\frac{1}{2})} - f^{(n-\frac{1}{2})})/\Delta_t = j\omega f^{(n)}$, we have a quadratic equation for $q = \exp(j\omega\Delta_t/2)$: $q^2 - (j\omega\Delta_t)q - 1 = 0$. The solutions are

$$q = \frac{j\omega\Delta}{2} \pm \sqrt{1 + \left(\frac{j\omega\Delta}{2}\right)^2}. \qquad (4)$$

If $|q| \leq 1$, FDTD fields are stable.

Hence, we conclude that all computed eigenvalues of the matrix A in (3) should hold two relations, $\mathrm{Re}(j\omega\Delta_t/R) = 0$ and $|\omega\Delta_t/R| \leq 2/\mathrm{R}$ for stable FDTD analysis.

4. Numerical Results

We consider a two-dimensional Lamé-mode resonator with side length L on an isotropic plate with Poisson's ratio $\sigma = 0.25$ in vacuum. **Figure 2** shows distributions of computed eigenvalues of (3) by the FDFD method run in the double precision arithmetic with $N = L/\Delta = 2^6$. The largest absolute values of the real parts of the eigenvalues computed by FDFD method run in the double and quadruple precision arithmetic are shown in **table 1**. The absolute values of the real part of the eigenvalues computed by FDFD method using an SSG model with stress imaging technique (SSGMSI) and three SGCV models, CSGCVM, SGCVMVF and SGCVMVD, are less than 3×10^{-10}, 4×10^{-5}, 2×10^{-9}, and 2×10^{-14}, respectively. These values computed in the quadruple arithmetic are smaller than 2×10^{-33}, that is approximately ten times the machine epsilon 1.9×10^{-34}, except for the values for the CSGCVM. In addition, using FDTD method run in the double precision arithmetic with a vibration source as a sine-modulated Gaussian pulse and $R = 0.5$, we confirmed that time

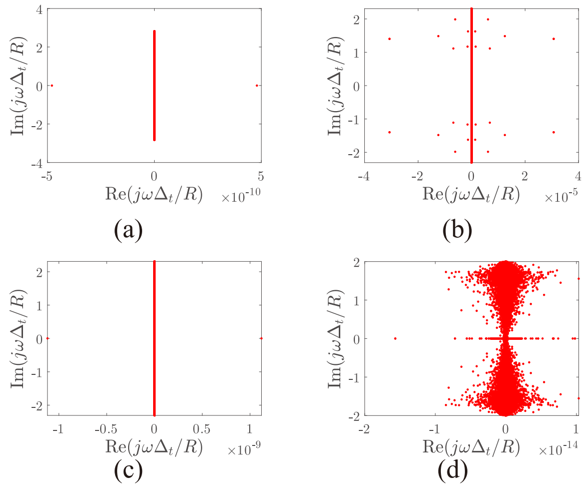

Fig. 2 Eigenvalue distributions computed by FDFD method with (a) SSGMSI, (b) CSGCVM, (c) SGCVMVF, and (d) SGCVMVD.

responses from $t = 0$ to $t = 2^{27}\Delta_t$ for the isotropic Lamé-mode resonator with SSGMSI and CSGCVM are stable and unstable, respectively. Hence, we can conclude that presented SGCV models, SGCVMVF and SGCVMVD, are stable.

Table 2 shows extracted parameters by fitting a function of N to computed eigenvalues, $\left(j\frac{\omega\Delta_t}{R}\right)(N) = \left(j\frac{\omega}{N\sqrt{2}}\frac{V_S}{V_P}\frac{L\sqrt{2}}{V_S}\right)(N) = j\frac{\omega}{N\sqrt{2}}\sqrt{(1-2\sigma)/(2-2\sigma)}\,(f_0 + f_p \times N^{-p})$, from $N = 2^4$, 2^5, 2^6, 2^7, and 2^8. These values show that accuracy of SSGMSI is better than SGCV models.

Table 1 The largest value of the real parts of the eigenvalues.

Model	Double	Quadruple
SSGMSI	2.9×10^{-10}	3.9×10^{-34}
CSGCVM	3.1×10^{-5}	2.1×10^{-5}
SGCVMVF	1.1×10^{-9}	1.3×10^{-33}
SGCVMVD	1.0×10^{-14}	1.0×10^{-33}

Table 2 Convergence parameters of the normalized fundamental resonance frequency.

Model	$f_0 - 1$	f_p	p
SSGMSI	5.4×10^{-8}	-0.4109	1.9998
SGCVMVF	-4.1×10^{-5}	0.4803	1.8975
SGCVMVD	5.4×10^{-6}	-0.3473	1.9690

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