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Stable modeling of free boundaries of an anisotropic plate resonator in the finite difference time domain method using staggered grid with collocated grid points of velocities

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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,[3,4] or staggered grids with the collocated grid points of velocities (SGCV).[5-7] 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 a stable SGCV model of free boundaries in two dimensions. Grid points of velocities are on the free boundaries for computing the integrals on control volumes for Newton's equation of motion rather than inducing stress-free conditions on the velocity fields[7] and unified approach to model interfaces between two, three, and four different media. The stability and validity of this model were demonstrated by computing resonant frequencies of a Lamé resonator on a quartz plate in the finite-difference frequency-domain (FDFD) method.

2. Stable SGCV Models of Free Boundaries

Figure 1 shows two SGCV models of free boundaries in two dimensions $(\partial/\partial z = 0)$. In Fig.1(a), we can compute extra velocities, v_a's (△), in the free boundaries and calculate after SGCV scheme in the solid.[7] In Fig.1(b), we compute a numerical integration of Newton's equation of motion by midpoint rule on the control volume (a rectangle with dashed lines) for velocities in the free boundaries: at the edge point, for example,

$$\frac{\Delta_x}{2}\frac{\Delta_y}{2}\,\rho\frac{\partial v_i(P_{ve})}{\partial t} = T_{ix}(P_{Tx})\frac{\Delta_y}{2} + T_{iy}(P_{Ty})\frac{\Delta_x}{2} \quad (1)$$

where Δ_i $(i = x, y)$, ρ, and T_{ij} $(i = x, y, z,\ j = x, y)$ are the space interval along i-axis, the mass

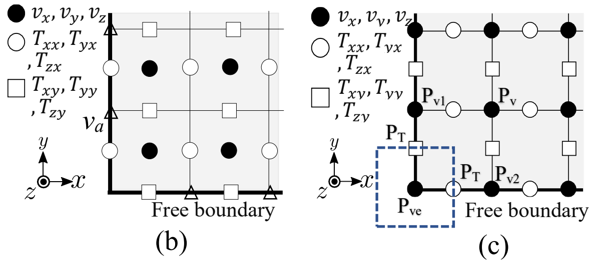

Fig. 1 stable SGCV models of free boundaries: (a) computing velocities in the free boundary,[6] (b) computing integrations on the control volume.

density, and an ij-component of stress tensor. In addition, using linear interpolation of velocity fields in the control volume with vertices, P_1, P_2, P_{ve}, and P_3, we can compute the time derivative of Hooke's law with the velocity gradient tensor Γ_{kl} at the grid points for T_{ij} as follows:

$$\frac{\partial T_{ij}(P_{Ty})}{\partial t} = \sum_{k,l} C_{ijkl}\,\Gamma_{kl}(P_{Ty}) \quad (2)$$

where C_{ijkl} is stiffness. The values of $\Gamma_{kl}(P_{Ty})$ can be computed by derivatives of linear fields of velocity in the control volume. Here, we assume that Γ_{kl} is a constant in the control volume.

3. Stability Analysis of FDTD Models

We used von Neumann stability analysis of FDTD models of a two-dimensional Lamé-mode resonator on a quartz 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

$$\frac{\partial}{\partial t}f^{(n)} = \frac{R}{\Delta_t}Af^{(n)} \quad (3)$$

where $R = V_N\Delta_t/\Delta_x$ is the Courant number, t, $f^{(n)} = \left[v^{(n)T}\,T^{(n)T}\right]^T$, A, and Δ_t are time, a field column vector composed of two column vectors, velocity column vector $v^{(n)}$ and stress-tensor column vector $T^{(n)}$ with discretized field values at all grid points, the normalized matrix of finite difference spatial operator, and a time interval. Here, the superscript (n) and T denote the values at the time $t = n\Delta_t$ and transpose of the column vector.

We used $V_N = (C_N/\rho)^{1/2}$ with C_N being the maximum value of the stiffness values.

Assuming that the elastic fields are time-harmonic fields with angular frequency ω, we have $f^{(n)} = f_\omega e^{j\omega n\Delta_t}$. Hence, we can derive an eigenvalue problem from (3) as follows:

$$j\frac{\omega\Delta_t}{R} f_\omega = A f_\omega \qquad (4)$$

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

Using the second order approximation of the time derivative in (3), $\partial f^{(n)}/\partial t \approx (f^{(n+1/2)} - f^{(n-1/2)})/\Delta_t = j\omega f^{(n)}$, we have a quadratic equation for $q = exp\left(j\omega\Delta_t/2\right)$: $q^2 - (j\omega\Delta_t)q - 1 = 0$. The solutions of this equation are

$$q = j\omega\Delta_t/2 \pm \left[1 + \left(j\omega\Delta_t/2\right)^2\right]^{1/2}. \qquad (5)$$

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

Hence, when all computed eigenvalues $(j\omega\Delta_t/R)$ of A in (4) are $\mathrm{Re}(j\omega\Delta_t/R) = 0$ and $|\mathrm{Im}(j\omega\Delta_t/R)| \leq 2/R$, the FDTD model is stable.

4. Numerical Results

We consider a two-dimensional Lamé-mode resonator with side length $l_x = 2na$ and $l_y = 2mb = 0.9673 l_x$ along the x and y axes on a quartz plate with Euler's angle (0°, −29.347°, 0°) in vacuum.[6] Here, we used the Bechmann's constants and ignored the piezoelectricity. **Figure 2** shows distributions of computed eigenvalues of (4) by the FDFD method run in the double precision arithmetic with $m = n = 1$ and $N = l_x/\Delta_x = l_y/\Delta_y = 2^6$. 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**. These values computed in the quadruple precision arithmetic are smaller than values in the double precision arithmetic and we can see that $\mathrm{Re}(j\omega\Delta_t/R) = 0$. Therefore, two FDTD models are stable.

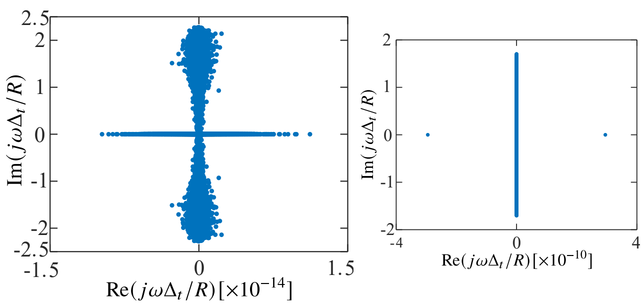

Fig.2 Eigenvalue distributions computed by FDFD method with free-boundary models (a) presented SGCV model, (b) rotated staggered grid (RSG) model[3,4] with grid points of stress components in the free-boundaries.

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

Model	Double	Quadruple
SGCV	1.1×10^{-14}	2.9×10^{-32}
RSG	3.0×10^{-10}	5.2×10^{-19}

Table 2 shows parameters extracted by fitting a function of N, $(j\omega\Delta_t/R)(N) = (j2\pi l_x f_c/V_N)(f_0/N + f_p \times N^{-p-1})$, to eigenvalues of (3) computed with $N = 2^5, 2^6, 2^7$, and 2^8. Here, f_c is the resonance frequency of the Lamé-mode and we use the extrapolated value from computed results by the COMSOL Multiphysics, $l_x f_c = 2400.24$ m/s. These values show that the RSG and SGCV models are comparable in accuracy.

5. Conclusions

A stable SGCV model of free-boundary with velocity grid points positioned in boundaries is developed for unified approach to model interfaces between two, three, and four different media. We demonstrated that this model is stable for modeling the interface between vacuum and an anisotropic solid.

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Table 2 Convergence parameters of the normalized resonance frequency.

Model	$f_0 - 1$	f_p	p
SGCV	-4.54×10^{-6}	0.907	1.91
RSG	-7.98×10^{-6}	1.45	1.96