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The Lattice Boltzmann Phononic Lattice Solid

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I present a Boltzmann lattice gas-like approach for modeling compressional waves in an inhomogeneous medium as a first step toward developing a method to simulate seismic waves in complex solids. The method is based on modeling particles in a discrete lattice with wavelike characteristics of partial reflection and transmission when passing between links with different properties as well as phononlike interactions (i.e., collisions), with particle speed dependent on link properties. In the macroscopic limit, this approach theoretically yields compressional waves in an inhomogeneous acoustic medium. Numerical experiments verify the method and demonstrate its convergence properties. The lattice Boltzmann phononic lattice solid could be used to study how seismic wave anisotropy and attenuation are related to microfractures, the complex geometry of rock matrices, and their couplings to pore fluids. However, additional particles related to the two transverse phonons must be incorporated to correctly simulate wave phenomena in solids.

KEY WORDS: Lattice solid; lattice gas; lattice Boltzmann; cellular automata; seismic waves; phonons.

1. INTRODUCTION

The lattice gas approach models fluids as a system of idealized gas particles that can move and collide on a discrete lattice. At the microscopic scale, the lattice gas physics is much simpler than the true physics of gas dynamics, yet the correct behavior encompassed by the Navier–Stokes equations is seen at the macroscopic scale.[(1)]

I present a first step toward the construction of a model with simplified microscopic physics capable of simulating macroscopic wave phenomena in complex solids. Ultimately, numerical experiments using such an approach could lead to an improved understanding of the how

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microscopic features and pore fluids in rocks affect seismic wave propagation.

For example, microfractures and grain alignments are known to cause seismic anisotropy,[2,3] although analyses are difficult due to the high level of geometric complexity in rocks.

Another example is the study of attenuation which is thought to be related to loss mechanisms such as fluid movements induced by seismic waves as they pass through porous rocks.[4] Several kinds of fluid may be present (oil, gas, water,...) whose behavior is nonlinear as well as viscous. Consequently, theoretical analyses are difficult due to the nature of the pore fluids coupled with the geometric complexity of rock matrices.

The lattice gas (LG) approach models phenomena including fluid flow,[5,6] flow in porous media,[7] constant-speed sound waves,[8] and multiphase fluid behavior.[9] A critical element required to model complex solids with a lattice gas-like method is an approach compatible with the LG method capable of simulating elastic vibrations in an inhomogeneous solid. This paper focusses on a first step enabling seismic P-waves to be modeled in *inhomogeneous* media using a lattice Boltzmann approach (note that earlier attempts at introducing inhomogeneity into both Boolean[10,11] and Boltzmann methods[12] tended to be without theoretical foundation or numerical verification). The key differences from the lattice gas method are (1) the introduction of a "scattering term" to the Boltzmann transport equation to encompass the wave scattering process which occurs at boundaries between materials with different properties (a lattice gas has only a "collision term"), and (2) the possibility of particle speed varying as a function of space.

The concept from solid-state physics of quanta of elastic vibration called phonons with both particle- and wavelike characteristics plays an important role, so I name the approach the "phononic lattice solid" (PLS) to distinguish it from the lattice gas (LG) approach for modeling fluids. I demonstrate theoretically and numerically that the phononic lattice solid models compressional waves in inhomogeneous media in the macroscopic limit.

2. PHONONS

A review of the principal properties of phonons helps to motivate the construction of the microphysics of the phononic lattice solid.

Quanta of elastic vibration called phonons[13,14] exist in infinite crystalline solids with a definite energy

$$E = \hbar\omega$$

and quasimomentum

$$\mathbf{p} = \hbar \mathbf{k}$$

which can be obtained by solving Schrödinger's equation

$$\hat{H}\psi = E\psi$$

and making use of the quantum condition (commutation relation)

$$\hat{p}_i \hat{q}_i - \hat{q}_i \hat{p}_i = -i\hbar$$

where carets are used to indicate operators and p_i and q_i are the momentum and position of the ith particle. The Hamiltonian for a solid has the form

$$H = T + V = \sum_{ij} \left(\frac{p_{ij}^2}{2m} \right) + \sum_{ij,i'j'} \left(q_{ij} q_{i'j'} \frac{\partial^2 V}{\partial q_{ij}\, \partial q_{i'j'}} + \cdots \right)$$

where the index i is used for the ith atom and the index j denotes the jth component of a vector. If the potential function is purely parabolic in the above Hamiltonian, phonons are noninteracting and pass through one another like classical elastic waves. Real interatomic potentials contain cubic and higher order terms, so displacements induced by one phonon are seen by other phonons as periodic variations in the medium properties (a kind of diffraction grating). Hence, phonons may be scattered from one another. This process can be analyzed using the formalism of second quantization,[15] which demonstrates that phonon interactions conserve the total quasimomentum to within any reciprocal lattice vector **b**. For example, a quartic term in the interatomic potential results in two-phonon interaction processes such that the sum of momenta of two incoming phonons equals the sum of momenta of two outgoing phonons. Hence, for a so-called normal process with $\mathbf{b} = 0$,

$$(\mathbf{k}_1 + \mathbf{k}_2)_{\text{after}} = (\mathbf{k}_1 + \mathbf{k}_2)_{\text{before}}$$

Thus, phonons interact in a way that is analogous to collision between classical particles.

There are three types of phonon, one dilational and two transverse, denoted the P, S1, and S2, respectively. This paper deals with the dilational particle only and focuses on the introduction of inhomogeneity. Future models will require transverse particle types to model the quasishear seismic waves as well as quasicompressional waves.

The particlelike property of collision will be combined with wavelike scattering behavior at medium boundaries to construct the phononic lattice solid. I make no attempt, or claim, to model phonons in a real solid as would be critical if studying the thermal properties of solids. Rather, my goal is to construct a simple microscopic world that correctly yields macroscopic wave phenomena in inhomogeneous media.

3. THE LATTICE GAS BOLTZMANN EQUATION

A brief review of the lattice Boltzmann lattice gas approach in two dimensions lays the ground for the phononic lattice solid.

Let $N_\alpha(\mathbf{x}, t)$ represent the number density of gas particles moving in direction $\alpha = [1,..., b]$. For particles moving with speed c, the Boltzmann transport equation is

$$\frac{\partial N_\alpha}{\partial t} + ce_{\alpha j}\frac{\partial N_\alpha}{\partial x_j} = \frac{dN_\alpha^C}{dt} \tag{1}$$

where dN_α^C/dt is the rate of change of number density in the α direction resulting from collision processes and $\mathbf{e}_\alpha$ is the unit vector pointing in the α direction. In a two-dimensional triangular lattice (i.e., $b = 6$), the unit vector $\mathbf{e}_\alpha$ is given by

$$\mathbf{e}_\alpha = (\cos([\alpha - 1]\, \pi/3), \sin([\alpha - 1]\, \pi/3]) \tag{2}$$

Equation (1) can be integrated using the first-order finite-difference (FD) equation

$$N_\alpha(\mathbf{x}, t + \Delta t) = N_\alpha(\mathbf{x}, t) - s[N_\alpha(\mathbf{x}, t) - N_\alpha(\mathbf{x} - \Delta\mathbf{x}_\alpha, t)] + \Delta N_\alpha^C(\mathbf{x}, t) \tag{3}$$

where $s \leqslant 1$ is the dimensionless particle speed measured as lattice spacings per time step, namely

$$s = c\frac{\Delta t}{\Delta x} \tag{4}$$

and $\Delta\mathbf{x}_\alpha$ is the vector between lattice sites in the α direction.

Equation (3) states that the number density of particles at the next time step $N_\alpha(\mathbf{x}, t + \Delta t)$ is the present number density $N_\alpha(\mathbf{x}, t)$ minus the fraction $sN_\alpha(\mathbf{x}, t)$ departing from the lattice site, plus an amount $sN_\alpha(\mathbf{x} - \Delta\mathbf{x}_\alpha, t)$ to account for particles arriving from the adjacent site, plus a term $\Delta N_\alpha^C(\mathbf{x}, t)$ to include the effect of collisions.

For a classical lattice gas the only nonzero dimensionless particle speed is unity, so Eq. (3) simplifies to

$$N_\alpha(\mathbf{x}, t + \Delta t) = N_\alpha(\mathbf{x} - \Delta\mathbf{x}_\alpha, t) + \Delta N_\alpha^C(\mathbf{x}, t) \tag{5}$$

(see also ref. 16). In this case, the time and space finite-difference errors cancel one another and the FD solution is exact.

By applying the Chapman–Enskog approach of expanding the N_α in terms of the macroscopic fluid velocity v_i and making use of conservation of mass and momentum, the form of the Navier–Stokes equations can be obtained in the macroscopic limit.[1] The viscosity depends on the details of the collisions and has been analyzed for both Fermi-like lattice gases[17] and Bose-like lattice gases.[18] The fermionic collision term has the form

$$\Delta N_\alpha^C = \sum_{S,S'} (S'_\alpha - S_\alpha) A(S \to S') \prod_\beta N_\beta^{S_\beta}(1 - N_\beta)^{(1-S_\beta)} \tag{6}$$

where the Boolean variables S_α and S'_α define input and output states, and $A(S \to S')$ is the transition probability from input state S to output state S'. Products with N_β evaluate the collision probability, while products with $(1 - N_\beta)$ compute the probability that the output state is not already occupied and is hence allowed (i.e., fermions obey the Pauli exclusion principle that only one particle is allowed in the same state).

For example, two incoming particles in the 1 and 4 directions represented as input state $S = [1, 0, 0, 1, 0, 0]$ may collide yielding two outgoing particles in the 2 and 5 directions represented as output state $S' = [0, 1, 0, 0, 1, 0]$. In the FHP-I lattice gas, the corresponding transition probability $A(S \to S')$ is 0.5, leading to a term in the sum $\sum_{S,S'}$ of form $\Delta N_\alpha^c = [-1, 1, 0, -1, 1, 0] \times 0.5 \times N_1 N_4 (1 - N_2)(1 - N_5)$.

4. THE LATTICE SOLID BOLTZMANN EQUATION

Consider wavelike particles representing elastic vibrations in a solid rather than classical particles of a lattice gas. The speed of elastic vibrations in a lattice depends on the elastic properties of the links (stiffness and density), which are allowed to be space and direction dependent. Therefore, the dimensionless speed must now be written as

$$s_\alpha(\mathbf{x}) = c_\alpha(\mathbf{x}) \frac{\Delta t}{\Delta x} \tag{7}$$

A vibration passing from a link with one property to a link with a different property is partially reflected and transmitted. The reflection and transmission coefficients for a particle moving in the α direction are denoted by $R_\alpha(\mathbf{x})$ and $T_\alpha(\mathbf{x})$. Vibrations are allowed to undergo phononlike interactions such that the number of particles and the quasimomentum are conserved (i.e., they undergo collisions like classical particles). The number density therefore obeys the lattice Boltzmann equation given by

$$N_\alpha(\mathbf{x}, t+\Delta t) = N_\alpha(\mathbf{x}, t) - s_\alpha(\mathbf{x})[N_\alpha(\mathbf{x}, t) - T_\alpha(\mathbf{x})\, N_\alpha(\mathbf{x}-\Delta\mathbf{x}_\alpha, t) - R_{\alpha+b/2}(\mathbf{x})\, N_{\alpha+b/2}(\mathbf{x}, t)] + \Delta N_\alpha^I(\mathbf{x}, t) \quad (8)$$

The interaction term denoted by ΔN_α^I is the same as the collision term for the Bose lattice gas ΔN_α^C, in keeping with the wavelike character of the particles. It has the form[18]

$$\Delta N_\alpha^I = \sum_{S, S'} (S'_\alpha - S_\alpha)\, A(S \to S') \prod_\beta N_\beta^{S_\beta}(1+N_\beta)^{S'_\beta} \quad (9)$$

The interpretation of Eq. (8) is similar to that of Eq. (3) except that the number of particles arriving from an adjacent site is modified by the transmission coefficient and an amount $s_\alpha R_{\alpha+b/2} N_{\alpha+b/2}$ is added to account for reflected particles. I have identified $N_\alpha(\mathbf{x}, t)$ with the number density of particles at time t *leaving* the lattice site at location $\mathbf{x}$. This explains why the transmission coefficient $T_\alpha(\mathbf{x})$ is present rather than $T_\alpha(\mathbf{x}-\Delta\mathbf{x}_\alpha)$.

Reflection and transmission coefficients for phonons are related through $1 = R_\alpha + T_\alpha$ (i.e., conservation of energy). However, the pressure of an inhomogeneous solid in equilibrium is constant, whereas the energy density is not. Therefore, I have chosen to deal with particles that carry a unit of pressure whose equilibrium distribution has the lattice gas form,[1,18] namely

$$N_\alpha^{\text{eq}} = \frac{p}{b}\left\{1 + \frac{D}{c^2} v_i c_{\alpha i} + G(p)\, Q_{\alpha ij} v_i v_j\right\} + O(v^3) \quad (10)$$

where p is the particle density, v_i is the macroscopic velocity of the solid, and $D = 2$ is the number of space dimensions. This choice allows lattice gas theory to be applied to the phononic lattice solid model with only minor extensions. I label the pressure particles pressions.

Reflection and transmission coefficients for pressions are related through

$$1 + R_\alpha = T_\alpha \quad (11)$$

(i.e., continuity of pressure) with the reflection coefficient given by

$$R_\alpha(\mathbf{x}) = \frac{Z(\mathbf{x}+\Delta\mathbf{x}_\alpha/2) - Z(\mathbf{x}-\Delta\mathbf{x}_\alpha/2)}{Z(\mathbf{x}+\Delta\mathbf{x}_\alpha/2) + Z(\mathbf{x}-\Delta\mathbf{x}_\alpha/2)} \quad (12)$$

where

$$Z = \rho c \tag{13}$$

is the acoustic impedence and ρ is the density of the medium.

The lattice solid Boltzmann equation can now be written as

$$\begin{aligned} N_\alpha(\mathbf{x}, t + \Delta t) = N_\alpha(\mathbf{x}, t) - s_\alpha(\mathbf{x})[N_\alpha(\mathbf{x}, t) - N_\alpha(\mathbf{x} - \Delta\mathbf{x}_\alpha, t)] \\ + \Delta N_\alpha^I(\mathbf{x}, t) + \Delta N_\alpha^S(\mathbf{x}, t) \end{aligned} \tag{14}$$

where

$$\Delta N_\alpha^S(\mathbf{x}, t) = s_\alpha(\mathbf{x})\, R_\alpha(\mathbf{x})[N_\alpha(\mathbf{x}, t) - N_{\alpha + b/2}(\mathbf{x}, t)] \tag{15}$$

is called the scattering term and accounts for the wave scattering processes. Note that the relation $R_{\alpha + b/2} = -R_\alpha$ was used to obtain this expression. Higher-order terms were dropped from the expansion $N_\alpha(\mathbf{x} - \Delta\mathbf{x}_\alpha, t) = N_\alpha(\mathbf{x}, t) + \cdots$ in passing from Eq. (8) to (15) to avoid errors from appearing in Eq. (21).

Hence, the phononic lattice solid Boltzmann equation (14) is the same as the lattice gas Boltzmann equation (3) except for the additional term ΔN_α^S.

The analysis is henceforth restricted to the case of inhomogeneous media with no intrinsic anisotropy (no crystal anisotropy) so $c_\alpha(\mathbf{x}) = c(\mathbf{x})$.

5. THE LATTICE SOLID MACROSCOPIC LIMIT

To first order, the lattice solid Boltzmann equation given by (14) corresponds to the Boltzmann equation

$$\frac{\partial N_\alpha}{\partial t} + c_{\alpha j} \frac{\partial N_\alpha}{\partial x_j} = \frac{dN_\alpha^I}{dt} + \frac{dN_\alpha^S}{dt} \tag{16}$$

where the term dN_α^S/dt is the rate of change of the number density due to scattering processes (partial reflection and transmission).

The macroscopic pressure P and velocity v_i are defined by

$$P \equiv \sum_\alpha \frac{N_\alpha}{D} \tag{17}$$

and

$$v_i \equiv \sum_\alpha \frac{N_\alpha e_{\alpha i}}{Z} \tag{18}$$

The assumed phononic behavior of particles (i.e., energy and quasimomentum conservation during interaction processes) implies the following constraints on the interaction term:

$$\sum_\alpha \frac{dN_\alpha^I}{dt} = 0 \tag{19}$$

and

$$\sum_\alpha \frac{dN_\alpha^I}{dt} e_{\alpha i} = 0 \tag{20}$$

which are the same as the conservation constraints for classical particles undergoing collisions.

Use is also made of the relations

$$\sum_\alpha \frac{dN_\alpha^S}{dt} = \sum_\alpha \left(\frac{N_\alpha e_{\alpha j}}{\rho} \frac{\partial Z}{\partial x_j} \right) \tag{21}$$

and

$$\sum_\alpha \frac{dN_\alpha^S}{dt} e_{\alpha j} = O \tag{22}$$

which can be verified by substituting the differential version of the reflection coefficient formula (12),

$$R_\alpha = \frac{Z(\mathbf{x} + d\mathbf{x}_\alpha/2) - Z(\mathbf{x} - d\mathbf{x}_\alpha/2)}{Z(\mathbf{x} + d\mathbf{x}_\alpha/2) + Z(\mathbf{x} - d\mathbf{x}_\alpha/2)} \to \frac{dx}{2Z} \frac{\partial Z}{\partial x_j} e_{\alpha j} \tag{23}$$

into the definition of the scattering term given by (15) and summing over direction α.

Summing the Boltzmann transport equation given by (16) over direction α and making use of the definitions (17) and (18) as well as the relations (19) and (21) yields the macroscopic equation

$$\frac{\partial P}{\partial t} + \frac{\rho c^2}{D} \frac{\partial v_j}{\partial x_j} = 0 \tag{24}$$

which can be integrated to provide the form of the classical relationship between pressure P and displacement u_j,

$$P = P_0 - \frac{\rho c^2}{D} \frac{\partial u_j}{\partial x_j} = P_0 - K \frac{\partial u_j}{\partial x_j} \tag{25}$$

where $K = \rho c^2/D$ is the bulk modulus of the medium.

The transport equation (16) multiplied by $e_{\alpha i}$ and summed over α yields a second equation. By applying the definition (18) and the relations (20) and (22), we can write the second equation as

$$\rho \frac{\partial v_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\sum_\alpha N_\alpha e_{\alpha i} e_{\alpha j}\right) = O \tag{26}$$

Expanding N_α in terms of the macroscopic velocity (Chapman–Enskog method) in the standard way[1] [see Eq. (10)] and using the moment relation

$$\sum_\alpha e_{\alpha i} e_{\alpha j} = b\delta_{ij}/D \tag{27}$$

and definition (17), we can simplify (26) to yield

$$\rho \frac{\partial v_i}{\partial t} + \frac{\partial P}{\partial x_i} = O(v^2) \tag{28}$$

By combining the macroscopic equations given by (24) and (28), one obtains [to $O(v^2)$] the wave equation for *inhomogeneous* acoustic media

$$\rho \frac{\partial^2 v_i}{\partial t^2} - \frac{\partial}{\partial x_i} K \frac{\partial v_j}{\partial x_j} = 0 \tag{29}$$

Hence, one sees that the Boltzmann transport equation (16) yields sound waves in an inhomogeneous medium with speed C related to the particle speed c through

$$C(\mathbf{x}) = \frac{c(\mathbf{x})}{\sqrt{D}} \tag{30}$$

In contrast, recall that a lattice gas yields constant-speed sound waves in a gas (i.e., waves in a homogeneous medium).

The analysis has aimed at including the effect of the scattering term (15). In order to correctly capture viscosity, one would require the v^2 terms in Eq. (28) which derive from the v^2 terms in the equilibrium distribution (10). However, a complete analysis is complicated by the presence of finite-difference errors when $s < 1$. In the special case of $s = 1$, Higuera's result for viscosity is applicable.[18] In general, the viscosity is expected to be isotropic in the macroscopic limit where the FD errors vanish.[19,20]

6. FINITE-DIFFERENCE SCHEME

The time evolution process specified by the lattice solid equation (14) consists of propagation, scattering, and interaction of the number densities $N_\alpha(\mathbf{x}, t)$. Propagation is analogous to the movement step in a lattice gas and can be achieved by using the first-order finite-difference scheme

$$N_\alpha(\mathbf{x}, t^*) = N_\alpha(\mathbf{x}, t) - s(\mathbf{x})[N_\alpha(\mathbf{x}, t) - N_\alpha(\mathbf{x} - \Delta\mathbf{x}_\alpha, t)] \tag{31}$$

The scattering step consists of adding the scattering term

$$N_\alpha(\mathbf{x}, t^{**}) = N_\alpha(\mathbf{x}, t^*) + \Delta N_\alpha^S(\mathbf{x}, t^*) \tag{32}$$

where the scattering term ΔN_α^S is specified by Eq. (15). The final step of interaction completes the time evolution process

$$N_\alpha(\mathbf{x}, t + \Delta t) = N_\alpha(\mathbf{x}, t^{**}) + \Delta N_\alpha^I(\mathbf{x}, t^{**}) \tag{33}$$

where the interaction term is specified by Eq. (9). The transition probabilities depend on the choice of collision rules. Particles represent vibrational quanta that cannot be brought to rest, so the FHP-I rules[1] are appropriate.

The entire time evolution process for the first-order lattice Boltzmann phonomic lattice solid consists of applying the three steps (31), (32), and (33).

For $s \leqslant 1$, the lattice solid transport equation (31) represents a stable first-order finite-difference scheme to solve the Boltzmann transport equation

$$\frac{\partial N_\alpha}{\partial t} + c_{\alpha j} \frac{\partial N_\alpha}{\partial x_j} = 0 \tag{34}$$

If $s = 1$, the time errors exactly cancel the space errors and the first-order finite-difference scheme yields the exact solution. However, if $s < 1$, errors of order $O(\Delta x, \Delta t)$ lead to numerical attenuation and dispersion of the solution for N_α.

For this reason, it is preferable to use a more rapidly converging second-order finite-difference scheme to perform the propagation step

$$\begin{aligned} N_\alpha(\mathbf{x}, t^*) = N_\alpha(\mathbf{x}, t) &- \frac{s}{2}(\mathbf{x})[N_\alpha(\mathbf{x} + \Delta\mathbf{x}_\alpha, t) - N_\alpha(\mathbf{x} - \Delta\mathbf{x}_\alpha, t)] \\ &+ \frac{s^2}{2}(\mathbf{x})[N_\alpha(\mathbf{x} + \Delta\mathbf{x}_\alpha, t) - 2N_\alpha(\mathbf{x}, t) + N_\alpha(\mathbf{x} - \Delta\mathbf{x}_\alpha, t)] \end{aligned} \tag{35}$$

This scheme corresponds to the predictor-corrector or Lax–Wendroff method[21] of the computational fluid mechanics literature. The second-order scheme is derived by truncating the Taylor series

$$N_\alpha(t+\Delta t)=N_\alpha(t)+\Delta t\frac{\partial N_\alpha}{\partial t}(t)+\frac{\Delta t^2}{2!}\frac{\partial^2 N_\alpha}{\partial t^2}(t)+\cdots \tag{36}$$

and expressing the time derivatives in terms of space derivatives by making use of the Boltzmann transport equation given by (34). Spatial derivatives are then calculated using centered finite-difference approximations.

The second-order scheme for propagation (35) followed by the scattering step (32) and interaction step (33) is referred to as the second-order lattice Boltzmann phononic lattice solid or second-order PLS.

For homogeneous media with $s=1$, the scattering term ΔN_α^S vanishes and the phononic lattice solid (to both first and second order) reduces to the classical lattice Boltzmann finite-difference equation for Bose fluid dynamics,[18] namely

$$N_\alpha(\mathbf{x}, t+\Delta t)=N_\alpha(\mathbf{x}-\Delta\mathbf{x}_\alpha, t)+\Delta N_\alpha^I(\mathbf{x}, t) \tag{37}$$

7. NUMERICAL EXPERIMENTS

Numerical experiments verify the phononic lattice solid (PLS) theory, which predicts isotropic P-waves in inhomogeneous media at the macroscopic limit. The tests demonstrate that the expected phenomena such as the reflected, transmitted, and conical waves are modeled by the PLS and that the solution converges.

Calculations were performed on a two-dimensional triangular lattice with the 1 and 4 directions aligned with the x axis [Eq. (2)] and using circular boundary conditions. The fully nonlinear collision operator with FHP-I rules was applied, but without triple collisions, to increase computing speed.

A scaled depth variable z' defined so that its integral values match those of lattice directions 2 and 3,

$$z'=z/\cos(\pi/3)$$

is displayed on plots.

8. WAVES IN INHOMOGENEOUS MEDIA

8.1. Two-Layer Model

Figure 1 depicts a snapshot of the vertical component of displacement computed using the second-order PLS at time step $t=350$ in a 500×400

grid. The medium consists of two horizontal layers whose interface was at $z' = 200$. The upper-layer particle speed was $c_1 = 0.5$ and the lower-layer particle speed was $c = 1.0$ with $\Delta t = \Delta x = 1$. A compressional source with a first-derivative Gaussian time history located at $(x, z') = (250, 170)$ excited waves with approximately 24 gridpoints per wavelength in the upper layer.

From top to bottom, the acoustic waves can be identified as follows:

- The upgoing direct wave in the upper layer at $(x, z') \approx (250, 70)$
- The upgoing reflected wave at $(x, z') \approx (250, 120)$
- The conical (refracted) wave at $(x, z') \approx (120, 180)$ and $(x, z') \approx (380, 180)$
- The downgoing transmitted wave at $(x, z') \approx (250, 340)$

For comparison, a simulation was made with the same model and source using a classical explicit second-order finite-difference (FD) scheme to solve the acoustic wave equation for inhomogeneous media. The FD result shown in Fig. 2 appears to be identical to the PLS result except for a perceptible level of background in the PLS solution. The background noise is present because the number density perturbations induced by the source were small (≈ 0.001) relative to the mean number density $d = 0.455$, thereby decreasing the effective precision of the PLS calculations.

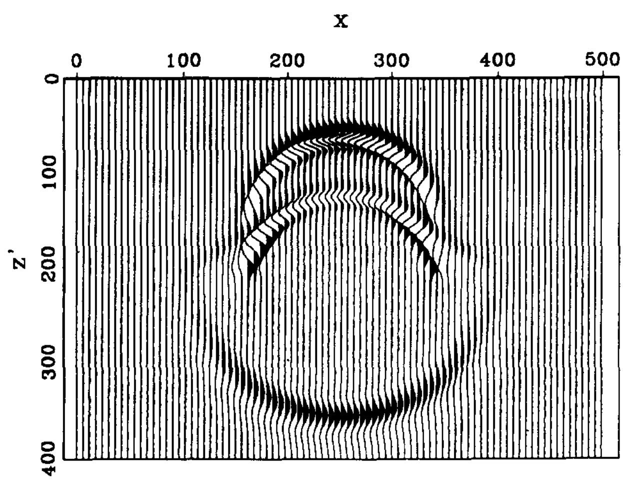

Fig. 1. Snapshot of the vertical component of displacement at time step $t = 350$ due to a compressional source at (250, 170) computed using the phononic lattice solid approach. The model consists of two horizontal layers with $c_1 = 0.5$ and $c_2 = 1.0$.

The finite-difference solution was subtracted from the lattice solid solution (Fig. 3) to highlight differences. These differences disappear in the macroscopic limit, where the lattice solid and finite-difference solutions converge to one another, as demonstrated in the following section.

8.2. Convergence

In this section, I study how the PLS solution converges to the classical FD solution, which is known to converge to the physical solution. Simulations were performed with the two approaches at various grid spacings relative to reference spacings $\Delta x_{\text{ref}} = 1$ and $\Delta t_{\text{ref}} = 1$ while fixing the particle speeds and source frequency in physical units (i.e., $\Delta t/\Delta t_{\text{ref}} = \Delta x/\Delta x_{\text{ref}}$ and $f_{\text{source}} = \text{const}$). For each grid spacing, the error between the two solutions is graphed to provide the rate of convergence.

Calculations are made in a two-horizontal-layer model with $c_1 = 0.5$ and $c_2 = 1.0$ and interface depth $z' = 0.55z'_{\text{max}}$. A horizontal plane-wave compressional source with a first-derivative Gaussian time history was initiated at time $t = 0$ and depth $z' = 0.40z'_{\text{max}}$. At the reference grid spacing, there are approximately six gridpoints per wavelength in the upper ($c_1 = 0.5$) layer. Note that although the calculations were made in two dimensions, the problem has one-dimensional symmetry and hence the results will be displayed as one-dimensional plots.

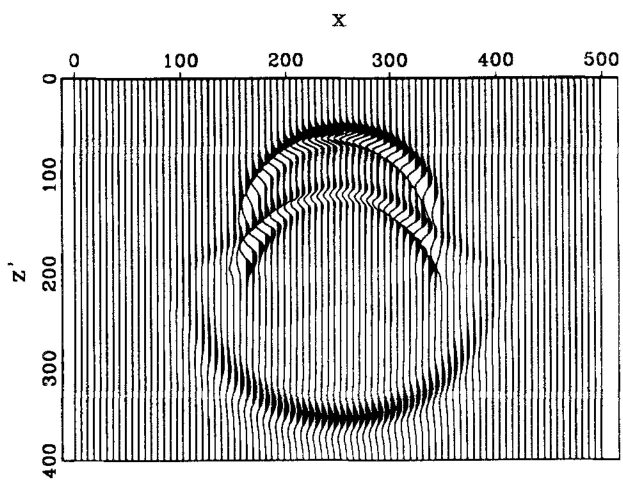

Fig. 2. Snapshot of the vertical component of displacement computed with the classical finite-difference method. The model, source, and plot parameters were identical to those used for the phononic lattice solid result.

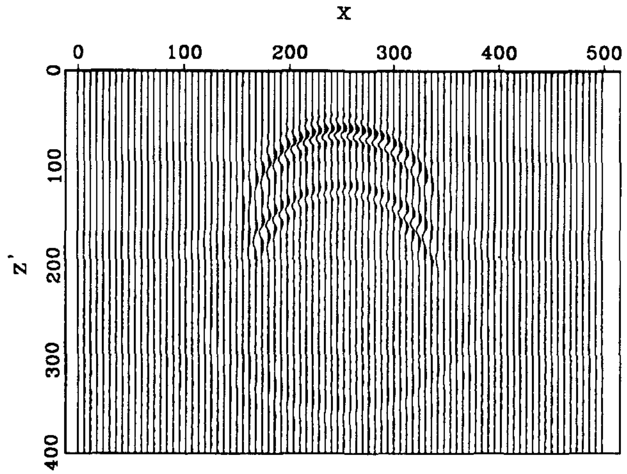

Fig. 3. The difference between the lattice solid and the finite-difference results ($LS-FD$) for the two-layer model.

Figure 4 shows a typical run made at 60 gridpoints per wavelength (i.e., $\Delta x = \Delta x_{\text{ref}}/10$).

The vertical component of displacement at time $t = 0.8 t_{\max}$ is graphed for ten grid spacings for the PLS and FD approaches in Fig. 5. The two solutions are similar when there are at least 24 gridpoints per wavelength. The differences, evident at larger grid spacings, are the result of finite-lattice effects and the characteristics of the Boltzmann and classical FD schemes.

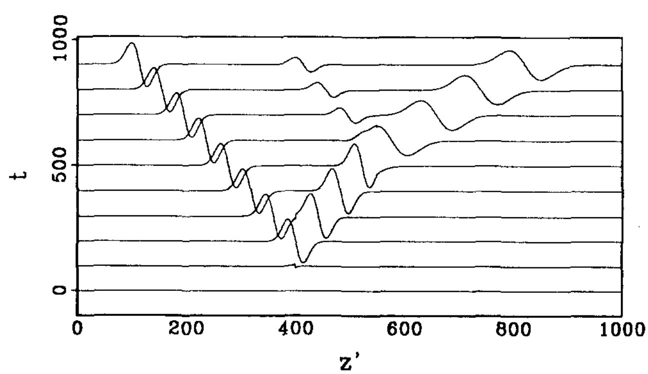

Fig. 4. Results of a typical lattice solid run used for the convergence calculations ($\Delta x = \Delta x_{\text{ref}}/10 \Rightarrow 60$ gridpoints per wavelength in the upper layer). The model is two horizontal layers with $c_1 = 0.5$ and $c_2 = 1.0$ and interface depth $z' = 0.55 z'_{\max}$. A plane wave source at depth $z' = 0.40 z'_{\max}$ was initiated at time $t = 0$.

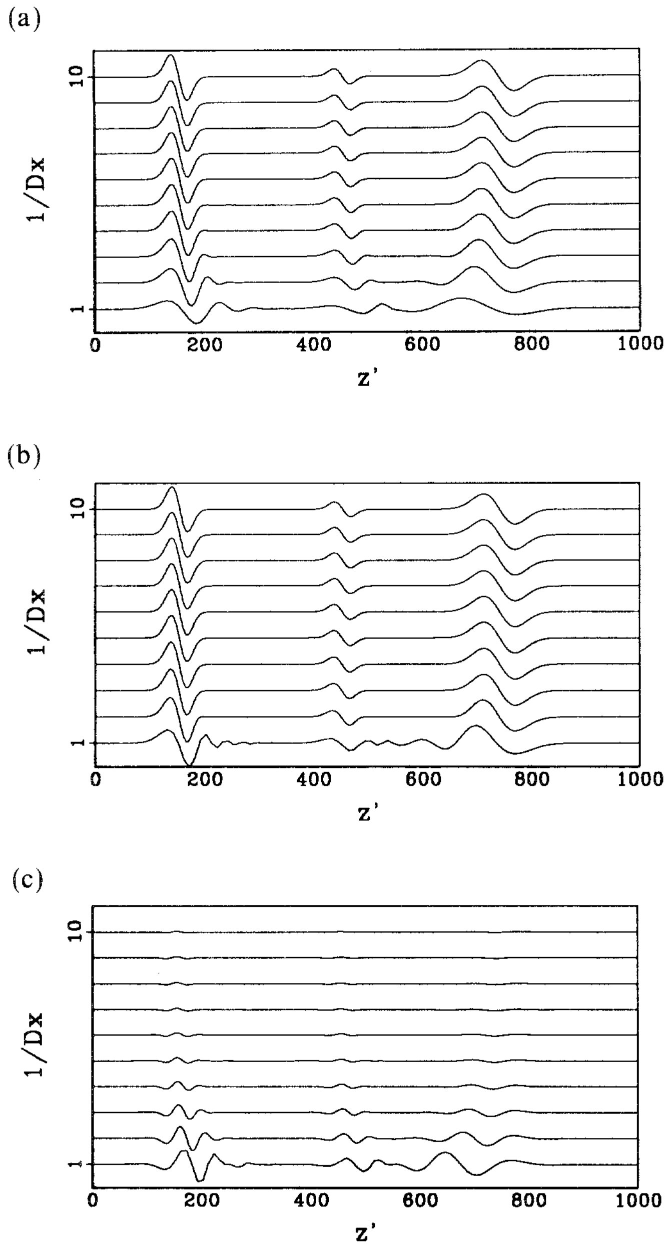

Fig. 5. The vertical component of displacement at time $t = 0.8t_{max}$ for ten simulations using the one-dimensional model and plane wave source with $\Delta x_{ref}/\Delta x = 1/\Delta x = [1,..., 10]$. (a) The second-order phononic lattice solid, (b) the classical second-order finite-difference method to solve the acoustic wave equation, and (c) the difference between the two solutions, $LS - FD$.

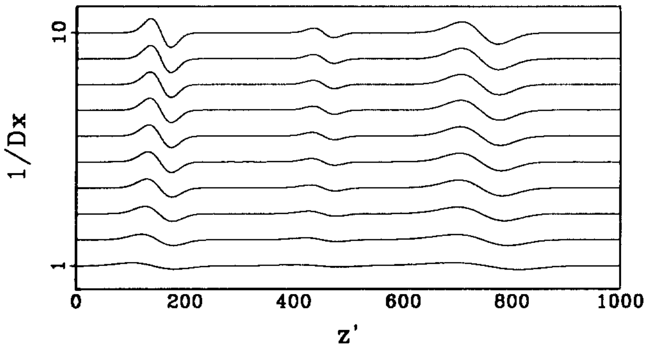

Fig. 6. The vertical component of displacement at time $t = 0.8t_{max}$ for ten simulations using the one-dimensional model and plane wave source with $\Delta x_{ref}/\Delta x = 1/\Delta x = [1, ..., 10]$ for the *first-order* phononic lattice solid, demonstrating its slower convergence.

The maximum error between the PLS and FD solutions at 24 gridpoints per wavelength is approximately 25%, as was the case in the two-dimensional example of Fig. 3. The error decreases to an acceptable level when there are 60 or more gridpoints per wavelength.

Runs were also performed using the first-order PLS approach to demonstrate its slower convergence relative to the second-order PLS (Fig. 6).

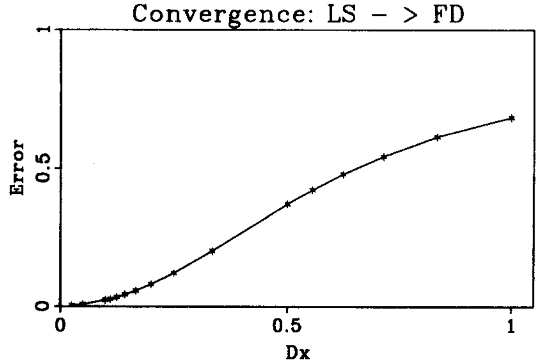

Fig. 7. The error between the second-order phononic lattice solid and finite-difference solutions. Near the origin, the error curve apparently tends to a parabola (i.e., $E \propto \Delta x^2$).

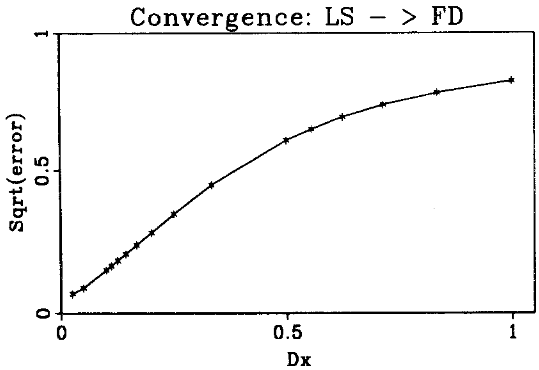

Fig. 8. The square root of the error between the second-order phononic lattice solid and finite-difference solutions. For small grid spacings (i.e., $\Delta x \in [0.1, 0.33]$ or 18–60 gridpoints per wavelength), the error curve is linear. Hence, $E \propto \Delta x^2$, as expected. The error is nonlinear for larger spacings because the high-order error terms (Δx^3, etc.) are significant. For small spacing ($\Delta x < 0.1$) the error is also nonlinear because of the finite computer precision which was responsible for the random noise evident in the two-dimensional snapshot.

Finally, the error between the two solutions is graphed as a function of the grid spacing, where the error is defined in the $L2$ norm as

$$E = \sum_t \sum_{z'} [u_z^{LS}(z', t) - u_z^{FD}(z', t)]^2$$

The second-order PLS and FD solutions should converge to one another as Δx^2, whereas the first-order PLS solution should converge to the second-order finite-difference solution as Δx. This is verified in Figs. 7–9.

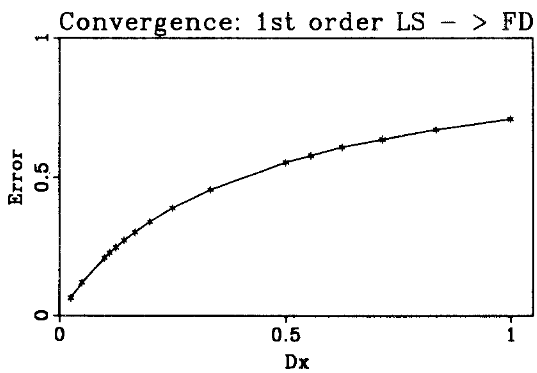

Fig. 9. The error between the first-order phononic lattice solid and second-order finite-difference solutions. Near the origin, the error curve seems to approach a line, so $E \propto \Delta x$, as expected.

9. CONCLUSIONS

An approach named the one-particle lattice Boltzmann phononic lattice solid (PLS) is developed to model seismic *P*-waves in inhomogeneous media at the macroscopic scale. It is similar to the lattice Boltzmann lattice gas method except that particle speed may vary in space and an additional term is added to the Boltzmann equation to include wave scattering processes. A theoretical prediction that pressure waves in an inhomogeneous medium are obtained at the macroscopic scale is verified numerically. The convergence rate is strongly dependent on the finite-difference scheme employed to solve the Boltzmann equation. The second-order PLS requires approximately 60 gridpoints per wavelength to obtain precise solutions. Ultimately, this approach could be used to study how seismic waves are affected by complex solids. However, the inclusion of additional particles related to the two shear phonons is required to model realistic solids which support shear waves.

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