

## Wavelet-based spatial and temporal multiscaling: Bridging the atomistic and continuum space and time scales

G. Frantziskonis<sup>1,\*</sup> and P. Deymier<sup>2</sup><sup>1</sup>*Department of Civil Engineering and Engineering Mechanics, University of Arizona, Tucson, Arizona 85721, USA*<sup>2</sup>*Department of Materials Science and Engineering, University of Arizona, Tucson, Arizona 85721, USA*

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A wavelet-based multiscale methodology is presented that naturally addresses time scaling in addition to spatial scaling. The method combines recently developed atomistic-continuum models and wavelet analysis. An atomistic one-dimensional harmonic crystal is coupled to a one-dimensional continuum. The methodology is illustrated through analysis of the dispersion relation, which is highly dispersive at small spatial scales and, as usual, nondispersive at large (continuum) scales. It is feasible to obtain the complete dispersion relation through the combination of the atomistic and the continuum analyses. Wavelet analysis in this work is not only used for bridging the atomistic and continuum scales but also for efficiently extracting the dispersion relation from the solution of wave propagation problems.

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### I. INTRODUCTION

Multiscaling has recently received increasing attention in several branches of physical science. In materials, a large part of the work is devoted to modern simulation methods involving coupling of length scales and sometimes time scales. Simulation methods for coupling length scales can be characterized as either serial or concurrent. In serial methods a set of calculations at a fundamental level (small length scale) is used to evaluate parameters for use in a phenomenological model at a longer length scale. For example, atomistic simulations can be used to deduce constitutive behavior of finite elements, which are then used to simulate larger-scale problems.<sup>1</sup> Several research groups are presently working productively on such methods, and several applications can be found.<sup>2-5</sup>

Concurrent methods rely on coupling seamlessly different computational methodologies applied to different regions of a material. For example, crack propagation is a problem that was tackled early on by multiscale methods.<sup>1,6</sup> Atomic simulation techniques (molecular dynamics) were used to model the crack tip where large deformations (even bond breakage) occur and continuum approaches [finite-element (FE) methods] were used to model the region far away from the crack tip.

Time scaling is of fundamental importance for many physical processes including diffusion or dynamics of macromolecular systems. These are systems with relaxation processes with vastly different scales (e.g., bond vibration versus macromolecule conformational change). Standard atomistic simulation methods are constrained by the shortest of these time scales. Surface diffusion has been addressed rigorously by Voter and co-workers (review paper<sup>7</sup>),<sup>8,9</sup> Here, based on transition-state theory, state-to-state transitions are obtained by several methodologies (accelerated dynamics methods such as hyperdynamics, parallel replica dynamics, temperature-accelerated dynamics), enabling the simulation of diffusion over extended time intervals. In Sec. V we briefly discuss possible connections of these works to the one

reported herein. We also note attempts to use wavelet analysis for detecting transitions, metastable structures, and for compressing data in such time-scaling works<sup>10</sup> and for molecular dynamics simulations of polymer chains.<sup>11</sup>

A novel multiscale method based on wavelets has been examined, up to now addressing spatial scales.<sup>12-15</sup> Here, the inherent capabilities of wavelet analysis to represent objects in a multiscale fashion are fully taken advantage of. The wavelet-based approach establishes a bridge between phenomena at different scales. Let us explain the process with respect to a “simple” material-related problem, i.e., consider a material for which porosity is the (only) source of heterogeneity and it manifests itself differently at various scales. For illustration purposes, consider a two-scale heterogeneity; at a scale large enough only the spatial distribution of “large” pores is observable, while at small scales that of the “small” pores can be seen. Even if the structure of the pores at these two distinct cases is fully specified or observed, it is difficult to compare the role of the porosity at each of the two scales on overall material properties. In other words, for, say, mechanical or electrical breakdown (failure), based solely on the spatial distribution of pores, it is difficult to decide whether the large or the small pores are of most importance. Furthermore, when the spatial scales extend beyond two orders of magnitude, numerical simulations become, in general, impossible (with present computers).

In order to identify the role of microstructure (two-scale porosity, extendable to more general cases) at each scale, consider the statistics of the wavelet transform of, say, the strain field for a deformation problem at one of the two scales. This information forms part of the wavelet transform of the entire medium, i.e., that consisting of pores at both distinct scales. By obtaining the wavelet transform at both scales and compounding them together, we have the statistics of the wavelet transform of the medium at all scales. This “compound” wavelet transform contains information on the entire medium, which can be used, for example, for crack initiation studies; it accounts for full interaction between scales. This process is used for identification of dominant scales<sup>13</sup> and is extended to a medium with pores and inclu-

sions at diverse scales.<sup>14</sup> Also, application to an aluminum alloy, A356, is demonstrated,<sup>14</sup> where the inclusions are the silicon particles, while the pores or oxides are at a scale much larger than those of the inclusions. Results from this work<sup>14</sup> agree well with recent experimental reports on crack initiation in A356 where the interplay of pores, inclusions, and boundaries is observed experimentally, yet not explained on a fundamental basis. A similar process has been used for studying grain growth at various scales by bridging a molecular dynamics (MD) and a Potts statistical model for grain growth, each applicable at two diverse range of spatial scales<sup>12</sup> and for self-affine media.<sup>15</sup>

In short, the wavelet-based multiscaling compounds the wavelet coefficients produced from the microstructure as it appears at each scale. The compounded information then characterizes the microstructure and relevant variables over a range of scales that is the union of the scales available.

This paper reports a study that extends the wavelet-based spatial multiscaling approach to temporal scaling. The major theme of the paper is time scaling. Recently developed atomic-continuum (AC) models are very effective in analyzing certain problems with spatial scaling, yet they do not—inherently—address time scaling. The herein reported combination of AC with wavelet analysis makes time scaling possible, and this furnishes the central contribution of this work.

The remainder of the paper first addresses issues about time scaling, then reviews the wavelet-based multiscaling method, and finally presents the approach to time scaling and results. The main purpose of the paper is to illustrate the time-scaling methodology, and this is done through a one-dimensional (1D) archetype problem. The existence of analytical solution for the problem examined herein, at both the atomic and continuum scales, helps greatly in illustrating and verifying the methodology in a lucid fashion. Extensions to other problems and the generality of the method are discussed towards the end of the paper.

## II. TIME SCALING ISSUES

Time scaling becomes important when the spatiotemporal scales to be linked in a multiscale framework extend from the atomic scale all the way to continuum ones. We first address why time scaling is important in such cases.

In continuum theories, the fundamental properties such as stress, strain, and constitutive parameters are thermomechanical quantities. These quantities are defined such that they satisfy the thermodynamic and long-time limits. That is, these quantities represent averages over a large enough number of atomic constituents and nearly infinite time. Calculating some of these quantities from atomistic models does not present significant difficulties as long as large enough systems and long enough times are used. Problems in bridging continuum, e.g., FE and atomistic regions may arise when the continuum or part of the continuum region is pushed outside the thermodynamic and long-time limits. This may be the case in many of the methodologies briefly reviewed above when the finite elements are reduced to “atomic” dimensions. Even when this is not the case, other problems are

present, and a clear demonstration of such problems has to do with dispersion relations, where the atomistic and continuum systems overlap only in the long wavelength limit.<sup>16</sup> Within the AC framework, atomistic simulations are used for identifying the constitutive behavior of the FE and it is difficult to extract the dispersion relation for scales (wavelengths) spanning from interatomic distances to macroscopic (continuum) ones. Thus, in the AC models, for example, there should be time scaling in addition to the dynamic feeding of information from small scales (atomistic) to large ones (continuum). In other words, for short time scales one should look at atomistic simulations and for long ones at continuum ones, with a rigorous coupling of time scales.

## III. WAVELET ANALYSIS AND THE COMPOUND WAVELET MATRIX

Wavelet analysis is key to this work, and there are several publications on this subject. A variety of different wavelet transforms exists, yet in every case the wavelets are derived from basic templates by taking scaled versions and putting them in many different positions; choosing an appropriate wavelet family for a specific problem is, in many respects, similar to choosing an appropriate finite element for a FE application. The complete family of an elementary function contains large scale and fine scale wavelets. The major advantage is that it enables one to see broad features on a wide scale while studying fine features one small piece at a time, so that the interaction between small and large-scale features can be studied.

In one dimension (extendable to higher ones) a wavelet  $\psi(x)$  transforms a fluctuating function  $f(x)$ <sup>17</sup>:

$$W_f(a,b) = \int_{-\infty}^{\infty} f(x)\psi_{a,b}(x) dx. \quad (1)$$

The two-parameter family of functions,  $\psi_{a,b}(x) = (1/\sqrt{a})\psi(x-b/a)$  is obtained from a single one,  $\psi$ , called the mother wavelet, through dilatations by the scaling factor  $a$  and translations by the factor  $b$ . The factor  $1/\sqrt{a}$  is included for normalization. The parameter  $a$  can take any positive real value, and the fluctuations of  $f(x)$  at position  $b$  are measured at the scale  $a$ . When discretized, wavelet analysis can be performed with fast algorithms.

Given the wavelet coefficients  $W_f(a,b)$  associated with a function  $f$ , it is possible to reconstruct  $f$  at a range of scales between  $s_1$  and  $s_2$  ( $s_1 \leq s_2$ ) through the inversion formula

$$f_{s_1,s_2}(x) = \frac{1}{c_\psi} \int_{s_1}^{s_2} \int_{-\infty}^{\infty} W_f(a,b)\psi_{a,b}(x) db \frac{da}{a^2} \quad (2)$$

and setting  $s_1 \rightarrow 0$  and  $s_2 \rightarrow \infty$ . A two-dimensional wavelet transform includes transforms in the  $x$  direction, the  $y$  direction, and in the diagonal  $x,y$  direction. For example, given an image of  $512 \times 512$  pixels, the wavelet transform consists of three  $256 \times 256$  matrices (one in each direction), three  $128 \times 128$  matrices, and so on; each decomposition level is at half the resolution from the previous one. The final level of decomposition represents the image at the coarsest resolution.

Given a function (e.g., the spatial distribution of a principal strain in a material with a hierarchical microstructure), its features over a range of length scales can be studied with wavelet analysis. Wavelets enable us to overcome the immense difficulty of performing numerical simulations on problems containing features at scales spanning more than two orders of magnitude. It is feasible, however, to perform appropriate simulations at various scales and thus obtain the function as it appears at these scales. The information gained at each of the scales is then used to synthesize the complete function.

The compound wavelet matrix (CWM) has been presented in detail elsewhere.<sup>12</sup> We briefly present the CWM here through an example relevant to the present work, for the sake of being as self-contained as possible; further, even though the example addresses spatial scaling only, it allows for an easily understandable transition to time scaling.

Let us consider a two-dimensional (2D) analysis for the purpose of illustration; it ends up that forming the CWM for 2D spatial analysis is conceptually equivalent to performing 1D spatial analysis with time scaling. At a coarse scale, a problem, e.g., the grain growth problem<sup>12</sup> or a wave propagation problem such as that presented in the following section, involving a “large” system is solved using continuum theories, e.g., FE. Next we consider a smaller system and the same problem is solved using molecular dynamics (MD). Within a statistical ensemble framework, the set of wavelet coefficients from each system represents the problem at two different scale ranges. However, the large system does not provide information on small scales and the small system does not provide information on large scales. Next the information gained from the large and small system is combined to form the “compounded wavelet matrix.” In 2D, the wavelet transform comprises of one in the  $x$ , one in the  $y$ , and one in the  $x$ - $y$  direction, as shown in Fig. 1; Fig. 1(a) shows (schematically) the wavelet coefficients, obtained from the relevant analysis of the smaller system and Fig. 1(b) shows those of the larger system.

Submatrix  $A$  shown in Fig. 1(b) represents details appearing at a certain discretization scale of the small system. The same discretization scale for the large system is shown as submatrix  $A$  in Fig. 1(b). By making the substitutions as indicated by the arrows, the compound matrix has information at those scales not “seen” by the larger system, yet seen by the smaller one. All the corresponding matrices (those with corresponding scale and discretization) are substituted; for simplicity, only three such substitutions are shown in Fig. 1. Hence, the compound matrix is a representation of the problem over a range of scales made by the union of the scales of the smaller and larger systems. Of course, the small-scale and the large-scale systems should have minimum overlap such that the full compound matrix can be built; this is addressed extensively elsewhere.<sup>12</sup> Alternatively, or equivalently, depending on the scales addressed by each system, the CWM can be built as shown in Fig. 2.

The process can naturally be extended to include time scaling. Consider a spatially 1D problem such as that described above. The CWM, as the ones in Figs. 1 and 2, can be built, but now the vertical axis is time, and the horizontal

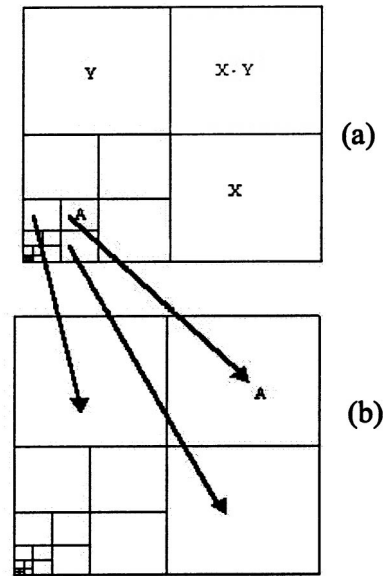


FIG. 1. Wavelet compound matrix: (a) wavelet coefficients from a small system; (b) from a large system. Arrows indicate the substitution of matrices in forming the compound matrix. Only three such substitutions are shown for illustration.

axis is the spatial variable of the problem. At large spatial and time scales [the “boxes” at the lower left corner of Fig. 1(b)], the compound matrix is filled in from the solution of the large system. At fine spatial and temporal scales, the solution of the small system fill in the relevant boxes [boxes in the upper right part of Fig. 1(b)]. The process is statistical and will yield full information on the problem at hand. The above process can be extended to higher spatial dimensions. For example, a spatially 2D can be addressed, but, now, the spatial/temporal compound wavelet matrix becomes three dimensional.

**IV. TIME SCALING ILLUSTRATION: DISPERSION RELATION**

The wavelet-based multiscale method is not like the AC ones, where information at large scales is fed from small

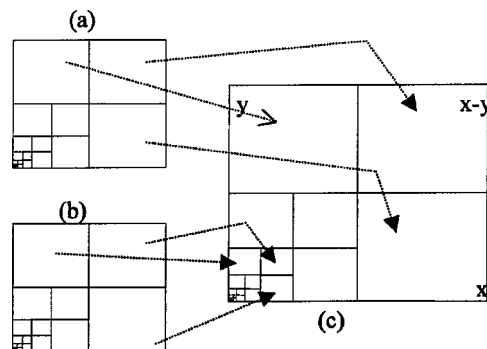


FIG. 2. (a) Wavelet coefficients from small system; (b) from large system; (c) CWM. For illustration, only a few schematic substitutions are indicated by the arrows in forming the CWM.

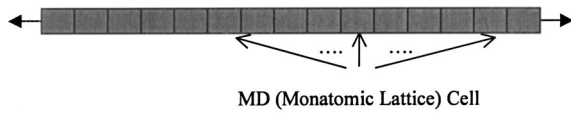


FIG. 3. An illustrative representation of a 1D system consisting of finite elements; the boxes represent finite elements, each corresponding to a monatomic lattice cell.

scales. The wavelet method possesses an important attribute, i.e., time scaling can be naturally embedded in the method, something very difficult to do using serial (AC) multiscaling. At the same time, when dynamic interaction between scales is appropriate, the wavelet method combined with AC ones provides a powerful multiscaling method. Here is what results by combining AC methods and wavelet-based ones, illustrated in this paper through dispersion relations; other problems can be handled similarly.

The concepts are herein implemented and demonstrated through 1D idealizations. For this purpose, a 1D FE dynamic analysis of a bar is combined with the so-called monatomic Bravais lattice analysis, appearing in solid state physics text books.<sup>16</sup> The Bravais lattice is in a sense a 1D molecular dynamics (MD) analysis tool and consists of a 1D chain of atoms each of mass  $M$  connected with linear springs of stiffness  $K$ . Figure 3 illustrates the problem.

The atomistic system in this case predicts a dispersion relation of the form

$$c(\omega) = \frac{a|\omega|}{\sin^{-1}[1 - (M/2K)\omega^2]}, \quad (3)$$

where  $a$  denotes the interatomic spacing,  $\omega$  denotes frequency, and  $c$  is the phase velocity of the wave. In solid state physics literature, usually the dispersion relation is expressed as the dependence of frequency on wave number. From that dependence for the monatomic lattice,<sup>16</sup> Eq. (3) can be easily derived. This relation yields  $c = \text{const}$  only for very small frequencies, i.e., in the continuum limit. The AC method cannot predict this kind of dispersion since the atomistic simulations are used in this case for obtaining the constitutive parameters. But, the combination of AC and wavelets analysis can.

Before presenting results, we comment that the process of combining wavelet analysis and AC does not change the AC process (minor adjustments to the size of the finite elements and the time steps for efficient overlapping in building the compound wavelet matrix should be implemented). The big difference with performing an AC analysis alone is that now information from the atomic system in each finite element is retained (in addition to the constitutive parameters) which is used in building the compound wavelet matrix.

The dispersion relation (3) for a monatomic lattice for a set of atoms of mass  $M$  distributed along a line at points separated by distance  $a$  and connected by springs of stiffness  $K$  is analytical. The goal of this paper is to compound information from the lattice and from continuum analysis in order to obtain the complete dispersion relation. Thus, we consider a problem such that in Fig. 3, that is too large to be solved by the atomic model. Yet, by compounding information from

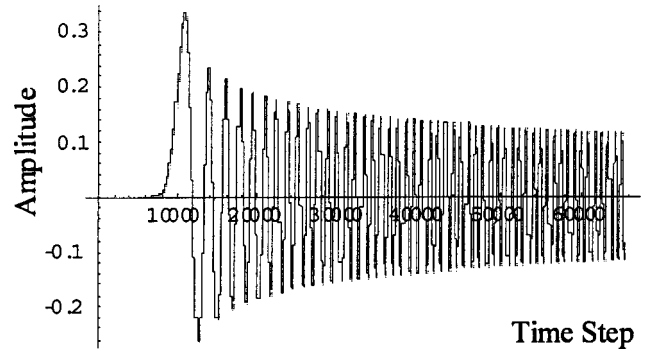


FIG. 4. Signal received at atom 1500 from the  $\delta$ -function excitation at atom 2000.

the atomistic and the continuum analysis, it is demonstrated here that the actual problem (large atomistic system) can be approximated satisfactorily.

Of course, for the illustrative purpose of this paper, we solve a large atomic system, and then verify that the compounded information from small atomic systems and continuum analysis can recover the dispersion relation.

## A. Results

### 1. Dispersion relation: Atomistic model

For the “large” atomic system we consider 4000 atoms in a monatomic lattice using periodic boundary conditions. Typically, the dispersion relation would be obtained from such a system by exciting a certain frequency at a point and receiving the traveling wave at another point. The arrival time would then provide the phase velocity for that specific frequency. Repeating the process for several frequencies would yield the dispersion relation. Here, however, we take advantage of the properties of the wavelet transform and avoid such a tedious process. We excite a point in a lattice by a  $\delta$ -function displacement, thus propagating all frequencies, receive the signal at some distance from that point and use wavelet analysis to deduce the dispersion relation.

We use unit values for  $K$ ,  $M$ , and  $a$ , and excite the atom at position 2000 by  $1 \times 10^{-3}$  units of displacement, for the first time increment only, i.e., we impose a  $\delta$  function at atom 2000. Using a time increment of  $5 \times 10^{-3}$  we receive the signal at the atom in position 1500. Figure 4 shows the received signal.

The signal contains  $65\,536 = 2^{16}$  points; thus there are 16 scales available. We use biorthogonal spline wavelets of order 10 and 4 (Ref. 17) and Fig. 5 shows the wavelet coefficients in scale versus time plot. Note that the majority of significant coefficients is concentrated in the lower (coarser) scales. Figure 6 shows the coefficients for scale 7 and scale 10.

Each scale in the wavelet transform represents the details that appear in the range from the previous scale to the next one. Thus, the wavelet coefficients, e.g., those in Fig. 7, represent the wave propagated within the corresponding range of frequencies. Then, since we have a range of frequencies, any velocity measured from such wavelet coefficients is the group velocity rather than the phase velocity of a fixed

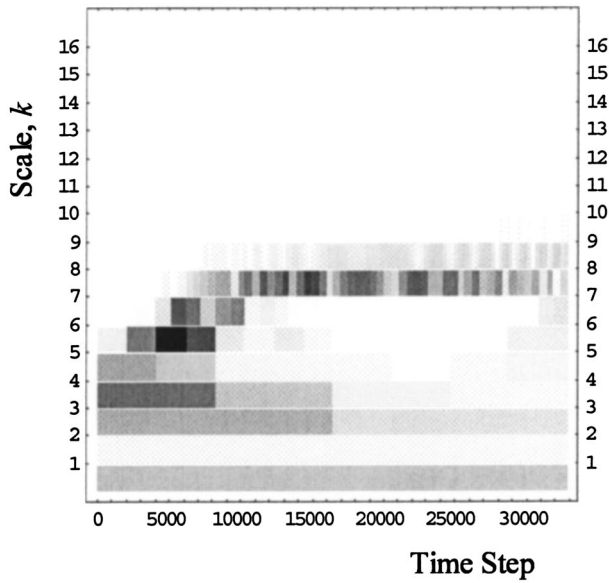


FIG. 5. Plot of the wavelet coefficients obtained from the signal shown in Fig. 4. The gray scale ranges from the maximum positive value (white) to the maximum negative value (black).

frequency.<sup>18</sup> In order to identify the dispersion relation from the wavelet coefficients, it is convenient to express it in terms of frequency as a function of the time of arrival of the signal at a fixed distance, proportional to  $1/c_g$ ,  $c_g$  denoting the group velocity. With  $S$  denoting such a fixed distance and for  $M, K$  equal to unity, the dispersion relation is expressed as

$$T_g/S = 1/c_g = \frac{1}{a\sqrt{1 - \frac{1}{4}\omega^2}}. \quad (4)$$

From the wavelet coefficients, we identify the first peak in the signal at each scale which exceeds a cutoff chosen to be  $10^{-9}$  for the present problem. This process leads to Fig. 7, where scale  $k$  (such that  $2^k \sim \omega$ ) is plotted against  $1/c_g$ . Note that for scales  $k$  greater than 14 the wavelet coefficients are practically null, indicating that the group velocities at the corresponding frequencies tend to zero, which is true when the wavelength approaches the interatomic distance  $a$ . Small scales (low frequencies) quickly approach the continuum limit where the group velocity is the same as the phase velocity; those waves arrive first as is clear from Fig. 7. Also, in Fig. 7 we compare the wavelet-based results to analytical ones (detailed above, i.e., Eqn. 4). At this stage it is noted that we have used the wavelet transform of a single wave propagation problem to identify the dispersion relation numerically. This process is severely advantageous to “usual” methods that solve a large number of wave propagation problems, i.e., at a large number of single frequency or narrow band pulses and measuring the time of arrival of the wave at a fixed distance.

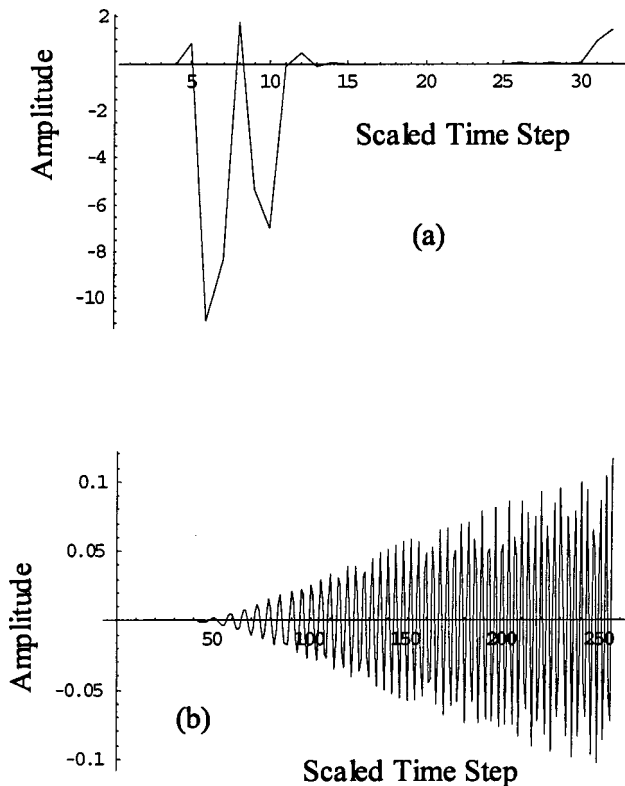


FIG. 6. Wavelet coefficients for scale 7 (a) and 10 (b).

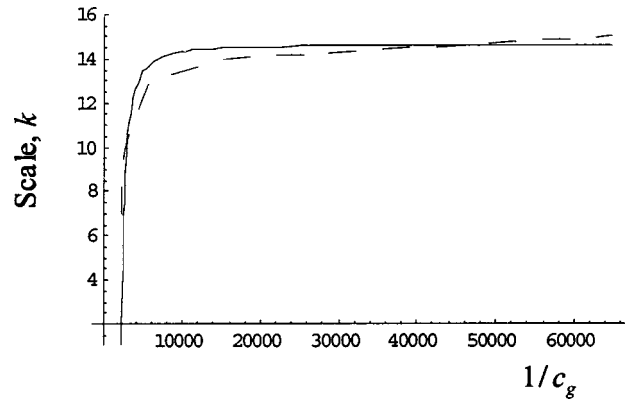


FIG. 7. Plot of scale  $k$  vs  $1/c_g$ . Dot line, as identified from the wavelet coefficients at several scales  $k$ . Solid line, from analytical solution.

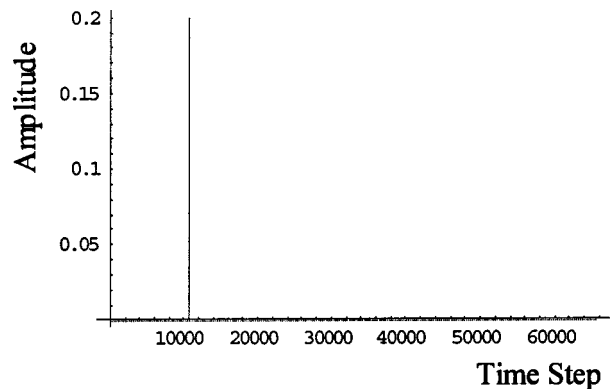


FIG. 8.  $\delta$ -function signal.

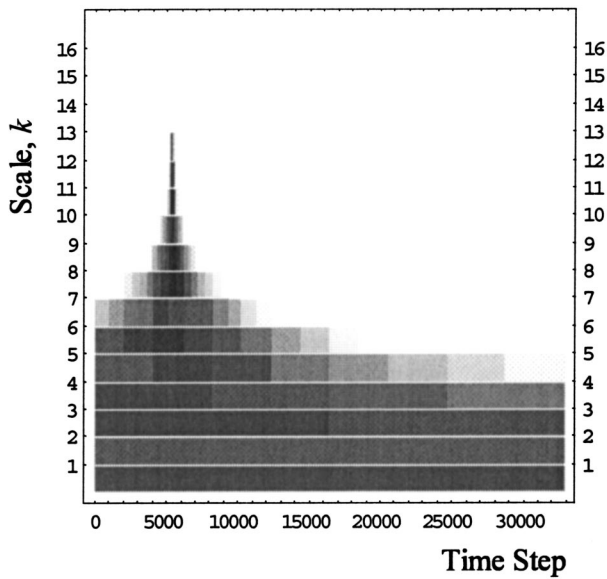


FIG. 9. Plot of the wavelet coefficients obtained from the signal shown in Fig. 8. The gray scale ranges from the maximum positive value (black) to the maximum negative value (white).

### 2. Dispersion relation: Continuum model

Continuum theories show no dispersion for homogeneous media, i.e., the phase velocity is identical to the group velocity and they are both independent of frequency. Thus, a delta function type of disturbance propagates as is. Numerically, we consider a problem similar to the one for the monatomic lattice above, but it is now solved within a continuum framework. For a homogeneous system, AC processes provide the needed elasticity modulus, a constant for the simple case at hand. It is interesting to see whether the wavelet analysis process captures the dispersion relation appropriately. We consider then a delta function signal arriving at the same fixed distance as in the monatomic lattice and perform the wavelet transform of the signal. For comparison, we utilize the same number of discretization points as in the monatomic lattice, and Fig. 8 shows the relevant signal.

Figure 9 shows the wavelet coefficients in scale time and Fig. 10 shows the coefficients for scale 8 and scale 10. Using the same process for identifying  $T_g$  as in the monatomic

lattice case, the wavelet coefficients yield a constant value of  $T_g$ , i.e., independent of scale  $k$ .

### B. Compounding the atomistic and continuum analyses

The atomistic and continuum analyses presented in the two previous subsections can be compounded as demonstrated in this section. The idea is that, in general, atomistic models address small systems (within the capability of computers) while continuum models address large ones. Thus, when a problem such as that of Fig. 3 is solved using an AC multiscale framework, the atomistic simulations in each FE can provide the variables needed for solution of the continuum (large) problem. For the illustration problem addressed herein, such a variable is the elasticity modulus. Yet, obtaining the dispersion relation of the medium, for example, would require solution of the entire or of a large enough medium (Fig. 3) using the atomistic model. This, however, is, in general, impossible; if it were possible, there would be no need to use AC processes. Of course, for the illustration purposes of this work a large atomistic one-dimensional system that yields the complete dispersion relation is solvable (Sec. IV A). Yet, we formulate and examine the compounding process for this problem in order to be able to compare results from a large atomistic system to those from information by compounding the atomistic and continuum system.

The CWM can be constructed as illustrated in Fig. 1 or 2, but now the vertical axis denotes time and the horizontal axis denotes the spatial variable of the problem,  $x$ . However, for the illustrative purpose of this paper, i.e., for determining the dispersion relation of the system, time scaling can be effectively demonstrated by compounding a signal such as that of Fig. 4 with that of Fig. 8. The extent of a signal, such as that in Fig. 4, depends on the size of the atomistic systems used, which are embedded in each of the finite elements, as well as on the number of time steps used in the atomistic system. Thus, the size of the atomistic system that can be solved efficiently dictates the size of the finite elements. Further, the total number of time steps used in the atomistic system must be such that the compound information yields the dispersion relation satisfactorily. This is explained further in the following.

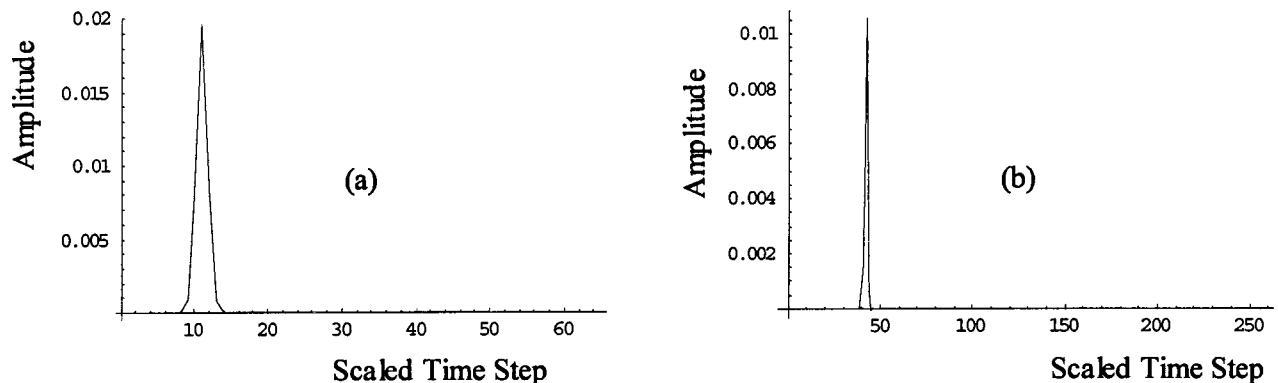


FIG. 10. Wavelet coefficients for scale 8(a) and 10(b).

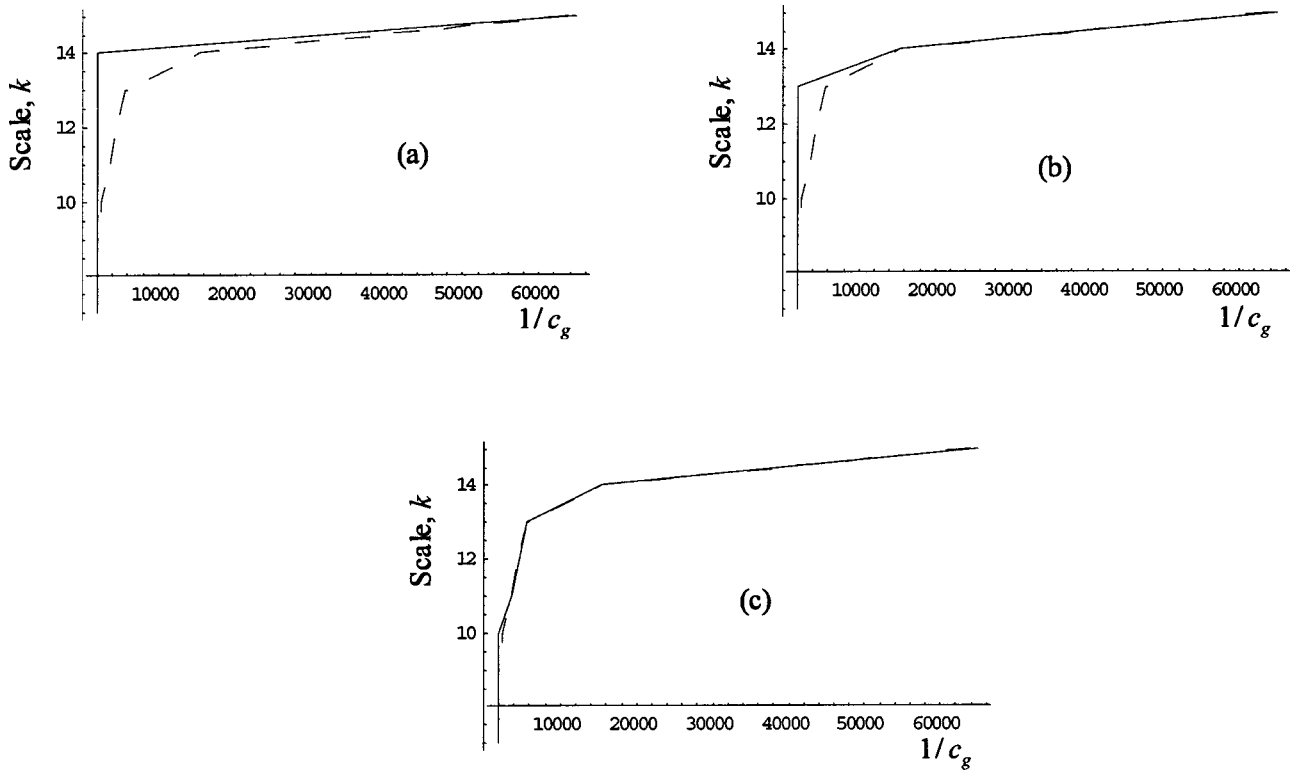


FIG. 11. Comparison of dispersion curve obtained from the compounded wavelet coefficients and that of Fig. 8. (a)  $m=12$ , (b)  $m=11$ , (c)  $m=8$ . Solid line, as identified from the compounding process. Dot line, as identified from the wavelet coefficients at several scales  $k$ , Fig. 8.

We compound the wavelet transforms, i.e., that of Fig. 5 and that of Fig. 9. For small scales  $k$  we use Fig. 9, and for large  $k$  we use Fig. 5. Let  $m$  denote the value of that scale such that for

$$k \leq m \tag{5}$$

the wavelet coefficients from the continuum formulation are used, and for

$$k > m \tag{6}$$

the wavelet coefficients from the atomistic system are used. The value of  $m$  depends on the time steps in the atomistic system which, in turn, depends on its spatial size (number of atoms) since the restriction here is computer power. For example,  $m=9$  implies that only time scales greater than 9 can be captured by the atomistic system, and for all lower time scales the continuum system applies.

Figure 11 compares the dispersion curve obtained from the compounded wavelet coefficients and that of Fig. 8. Note that the above process of compounding wavelet coefficients is not statistical, as would be the general case, e.g., dealing with problems in higher spatial dimensions with nonhomogeneous material structure. For the homogeneous material case examined, and for the dispersion relation, it is possible to perform the inverse wavelet transform of the compounded wavelet coefficients and thus obtain a signal, i.e., the received wave at a certain position. Figure 12 shows the signal evaluated this way for  $m=8$ . The correlation coefficient between this signal and that of Fig. 4 has also been evaluated

and it was found to be 0.897 (correlation coefficient equal to 1 indicates identical signals). Some of the high amplitudes are “filtered out” in the process, yet, overall, the basic characteristics of the signal are reconstructed well. For  $m=11$  this correlation coefficient reduces to 0.528, and for  $m$  larger than that the coefficient of correlation drops quickly.

### V. CONCLUSIONS, EXTENSIONS, LIMITATIONS, AND FUTURE WORK

Wavelets and the formation of the compound wavelet matrix allow for a natural way to address time scaling within a spatiotemporal multiscale framework. This is illustrated in the present paper by addressing the dispersion relation in an atomistic and in a continuum system, both in one spatial

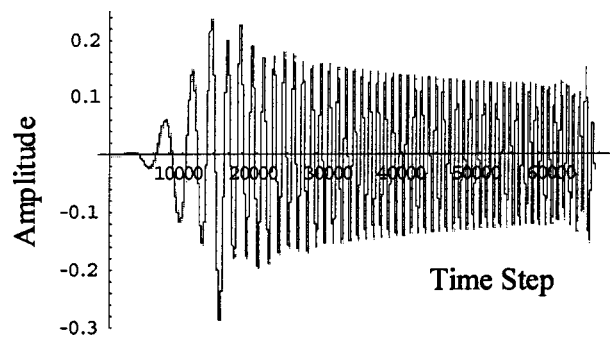


FIG. 12. Signal produced by the inverse wavelet transform of the compounded wavelet coefficients for  $m=8$ .

dimension. Even though this problem is relatively simple to address, especially since the analytical expression for the dispersion relation is known, the purpose of the paper is to illustrate the time scaling process. When dynamics are important, the method can be naturally combined with AC models. The process of combining wavelet analysis and AC does not change the AC process (minor adjustments to the size of the finite elements and the time steps for efficient overlapping in building the compound wavelet matrix should be implemented). The big difference with performing an AC analysis alone is that now information from the atomic system in each finite element is retained (in addition to the constitutive parameters) which is used in building the compound wavelet matrix. The process is extendable to nonhomogeneous systems in one and higher spatial dimensions, where the statistical nature of the process and the problems it addresses has to be stressed. Obvious extensions are higher spatial dimensions for wave propagation problems with applications in shock-wave physics, nondestructive material evaluation, high frequency acoustic microscopy, acoustic medical imaging, etc. In addition to wave propagation, the wavelet-based approach presented here can address several physical problems where vastly different time scales play an important role. We briefly discuss such an extension to the simulation of diffusion in particular. Diffusion problems can often be studied with molecular dynamics (MD) where com-

puter power limits the time and spatial scales to relatively small ones. At the same time, continuum diffusion theories can address problems of larger spatiotemporal scales; in addition, MD simulations can feed information to the continuum theories dynamically. As noted in this paper, bridging atomistic time scale to continuum time scales using the CWM method requires that there is overlapping in space and time between the atomistic and the continuum simulations. Forcing the continuum discretization to atomic scales may lead to unrealistic behavior. In contrast, accelerated atomistic simulation techniques<sup>7-9</sup> could be used efficiently with the wavelet-based multiscale methodology. These accelerated techniques can reach simulation times up to seconds or even hours in certain cases.<sup>9</sup> Achieving time overlap between accelerated atomistic simulations and continuum diffusion models provides the necessary condition for applying the CWM method to diffusion problems. The wavelet-based approach will then yield a model of diffusion from the atomic, to large structures spatial and temporal scales.

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\*Electronic address: frantzis@email.arizona.edu

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