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Homogenizing atomic dynamics by fractional differential equations

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ABSTRACT

In this paper, we propose two ways to construct fractional differential equations (FDE) for approximating atomic chain dynamics. Taking harmonic chain as an example, we add a power function of fractional order to Taylor expansion of the dispersion relation, and determine the parameters by matching two selected wave numbers. This approximate function leads to an FDE after considering both directions for wave propagation. As an alternative, we consider the symbol of the force term, and approximate it by a similar function. It also induces an FDE. Both approaches produce excellent agreement with the harmonic chain dynamics. The accuracy may be improved by optimizing the selected wave numbers, or starting with higher order Taylor expansions. When resolved in the lattice constant, the resulting FDE's faithfully reproduce the lattice dynamics. When resolved in a coarse grid instead, they systematically generate homogenized algorithms. Numerical tests are performed to verify the proposed approaches. Moreover, FDE's are also constructed for diatomic chain and anharmonic lattice, to illustrate the generality of the proposed approaches.

1. Introduction

Atomic motion is represented by displacement away from equilibrium. In a crystal solid, equilibria positions of all atoms form a periodic structure in space, called atomic lattice. The smallest repeating structure is a unit cell. Besides external forces, atomic motion is driven by interatomic potentials, including pairwise ones, three-body ones, etc. These potentials induce interatomic forces acting upon the atoms. Atomic/molecular dynamics simulations calculate resulting Newton equations. If one resolves the dynamics accurately, then complete description for the physical system is obtained. In this way, atomic simulation suits well to explore physical properties and mechanical behaviours, particularly for systems at microscopic scale, ranging from thermal conduction in nonlinear chains to failure in golden nanowires [1,2].

Atomic/molecular dynamics simulations nowadays offer a standard toolkit for exploring physical/mechanical processes in nano- or micro-scales. In a larger scale, however, full atomic dynamics require immense computing power, which is too expensive or even formidable. Multiscale simulations may remedy this difficulty and effectively capture features at both fine and coarse scales, if the atomic dynamics causes either a homogenized effect, or a localized effect in one or several fine scale subdomains. In the former case, homogenization is usually performed rigorously or heuristically by certain asymptotic expansions, and leads to coarse scale differential equations at the continuum level. See [3–6]. In the latter case,

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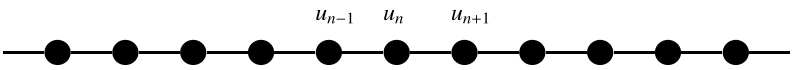

Fig. 1. Schematic plot of harmonic chain.

homogenization is also necessary for efficiently simulating the vast coarse scale domain complimentary to the selected fine scale subdomains.

On the other hand, the development of fractional derivative dated back to the early years when Newton and Leibnitz invented differential and integral calculus. Unlike standard calculus, there are various definitions for fractional derivative, including those named after Caputo, Riemann–Liouville, Grunwald–Letnikov, etc. [7]. The most distinct feature of fractional derivative is its integral-differential form with convolution. While causing difficulty in numerical resolution, this globality also facilitates modeling of applications with long time/space correlations. For instance, anomalous diffusion characterized by certain Brownian motion may be described by such an equation [8]. More applications can be found in rheology, brain aneurysm, visco-elasticity, fluid-structure interaction, just to name a few [9–11].

In a previous study for concurrent multiscale algorithm, we proposed to coarsen the atomic dynamics by matching Taylor expansions (matching differential operator approach) [12]. In case of a linear chain, this is actually equivalent to matching the dispersion relation by polynomials. We extend this idea, and propose here to match the dispersion relation with the help of functions of fractional power. This naturally induces a fractional differential equation (FDE). When the FDE is resolved precisely with the lattice constant as the space grid size, the linear chain dynamics is reproduced almost exactly, which is guaranteed by the Parseval's relation. When resolved over a coarse grid, the FDE resolution is determined by the Nyquist law. This in turn provides an accurate approximation for the atomic dynamics under this resolution. Along this line, we further propose to match the symbols of the force term in the Newton equation. Again the dispersion relation is approximated at high accuracy. The numerical discretization of FDE in space is performed with an algorithm of spectral accuracy [13].

The proposed approaches apply to more general lattices. We illustrate in the appendices for a diatomic chain and an anharmonic chain as examples. For the diatomic chain, we obtain two set of approximate FDE's. By matching the dispersion relations, we obtain averaged equations for the mean motion and relative (inner-molecular) motion, in a decoupled manner. By matching the symbols, we obtain coupled coarse scale equations for the heavy atoms and light atoms, respectively. For the anharmonic chain, only by matching symbols can we obtain a homogenized FDE.

The rest of this paper is organized as follows. In Section 2, we first describe the linear harmonic chain model, and introduce the fractional derivatives. Then we design FDE's to approximate the dispersion relation, and the symbol respectively, of the atomic model. In Section 3, we describe how to obtain coarse grid dynamics by semi-discretisation of the resulting FDE via centered differences. In Section 4, we first illustrate the accurate approximation by comparisons of the dispersion relations for the original Newton equation and the constructed FDE's. Then we perform time integration and demonstrate the effectiveness by numerical examples. Some concluding remarks are made in Section 5. In the appendices we further extend the approaches to homogenize diatomic chain and anharmonic chain.

2. Harmonic chain and approximate FDE's

We consider a monatomic chain shown in Fig. 1. The lattice constant is h_a, and the atom mass is m. The displacement of n-th atom away from its equilibrium is denoted as $u_n(t)$. For simplicity, nearest neighboring interaction is assumed. The interatomic potential between atoms numbered $(n-1)$ and n is $V(h_a + u_n - u_{n-1})$. The governing Newton equation then reads

$$m\ddot{u}_n = -\partial_{u_n}\left[V(h_a + u_n(t) - u_{n-1}(t)) + V(h_a + u_{n+1} - u_n)\right]. \tag{1}$$

We make a harmonic approximation of the potential, namely, $V(r) = \frac{1}{2}Er^2$, and rescale space by h_a, time by $\sqrt{m/E}$. This gives the harmonic chain with

$$\ddot{u}_n = u_{n-1} - 2u_n + u_{n+1}. \tag{2}$$

In the following, we construct FDE's corresponding to the Newton equation (2).

Two methods are proposed. First, we notice that the dynamics for a linear lattice is characterized by its dispersion relation, expressed in terms of trigonometric function. A function of fractional power is added upon the low order Taylor expansion, with the parameters determined by matching two selected wave numbers. An FDE is then obtained by considering the derivatives corresponding to the square of the approximate dispersion relation. Alternatively, we may also consider the symbol of the force term in the Newton equation, which is also expressed in terms of trigonometric function. Making an approximation in the same fashion, we may construct another FDE. This symbol matching also leads to an approximation of the dispersion relation, yet in a different form.

When a space discretization is performed with grid size the same as the lattice constant ($h_a = 1$ in this rescaled Newton equation), the matching of the dispersion or the symbol naturally induces an accurate approximation of the lattice dynamics. In the mean time, if resolved in a larger grid size, the semi-discretized FDE systematically provides coarsening for the lattice dynamics.