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Spatial filters for bridging molecular dynamics with finite elements at finite temperatures

S.B. Ramisetti, G. Anciaux *, J.F. Molinari

Ecole Polytechnique Fédérale de Lausanne (EPFL), School of Architecture, Civil and Environmental Engineering (ENAC), Computational Solid Mechanics Laboratory (LSMS), 1015 Lausanne, Switzerland

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ABSTRACT

We present the application of digital filters to split the energy spectrum of an atomistic zone simulated with molecular dynamics into low and high energy components. After a brief background on digital filters, we describe the procedure used to select a cutoff frequency for the filters. Then, a one dimensional numerical model based on the generalized Langevin equation (GLE) is used to study the system dynamics. We tested both time and spatial filters for the frictional term in GLE. Our results demonstrate that spatial filters are better than time filters to perform a selective damping within a molecular dynamics zone. Two dimensional examples validating our approach are also presented. Spatial filters should thus be favored in finite-temperature direct-coupling methods between molecular dynamics and finite elements.

1. Introduction

Several materials science and mechanical problems are multiscale in nature. It is known that the macroscopic material properties depend on various processes occurring at different length and time scales [1–3]. Examples of relevance to engineering include crack nucleation, crack propagation and friction [4–7]. For instance, in the case of sliding contact, the frictional forces between two materials are due to various physical mechanisms like long range elastic deformations, plasticity, third body interactions, asperity locking, heat transfer and lattice dynamics [8]. It has been shown that the atomistic processes play a critical role on the global behavior of friction [9,10]. It is also known that the heat transfer occurring across the sliding interface is due to frictional heating and plasticity which indeed are due to the atomic interactions [11,12]. However, the macroscopic interactions like the long range elasticity and plasticity are important to be considered in order to capture the atomistic processes accurately. Thus, there is a need for multiscale models coupling different length and time scales allowing to simulate material behavior. This has generated an intense development towards the research of multiscale methods [13–16].

During the past decades, several multiscale approaches have been developed to investigate material problems. There exist different methods such as finite element atomistics method (FEAt) [17], quasicontinuum method (QC) [18,5], coupling of length scales (CLS) [19], coupled atomistic and discrete dislocation (CADD) [20], bridging scale method (BSM) [21] and bridging domain method (BD) [22]. A broad classification of multiscale approaches into hierarchical and direct multiscale methods is done in [3]. In hierarchical methods, different scales are modeled separately and the information from the fine scale is passed to the coarse scale. This approach avoids the technical difficulty of direct coupling between scales, which explains the reason for its wide usage. However, the main drawback of this approach is the separation of scales assumption, which is often a too strong approximation for real applications. In direct or concurrent multiscale approaches, simulations at different length scales are performed simultaneously. For instance, fine scale or atomistic models like molecular dynamics (MD) are used in the critical regions to capture atomistic processes, while coarser or continuum models like the finite element (FE) method are used in the regions away from the complex atomic behavior. The coherency between the two models is enforced in an interface or overlap region, where both atomistic and continuum models coexist. The remainder of this article is built targeting the direct FE-MD coupling strategies.

One of the major problem with the concurrent coupling strategies is the spurious reflection of high frequency waves at the interface or overlap region. Depending on the coupling strategy employed, the amount of these reflections varies. At low temperatures, most coupling strategies have been thoroughly studied to prevent these spurious reflections [22,23]. However, it is difficult to use these methods at high temperatures due to the presence of unavoidable high frequency modes within the system. For

* Corresponding author.
E-mail address: guillaume.anciaux@epfl.ch (G. Anciaux).

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instance, it was shown that it is difficult to use the bridging domain method at finite temperatures above hundreds of Kelvin [24]. The bridging domain method is based on a projection of the atomic degrees of freedom on the coarser description. By projection techniques, we mean that the atomic degrees of freedom are "glued" with the continuum nodes. This is different from the bridging scale methods, where no overlap is considered and thus no direct projection of the atomic description onto the continuum is used. To the best of our knowledge, some attempts at developing concurrent multiscale methods treating thermal effects have been made, but with limitations [25–29]. Indeed, the main challenge lies within the modeling of heat transfer using MD. Heat transfer is a physical process that occurs due to energy transport carriers such as phonons and electrons [30]. At the continuum length scale, mechanical and thermal models can be clearly distinguished using two partial differential equations with no loss of accuracy. Whereas at the atomic length scale, both mechanical and thermal information are inherent within atomic velocities and cannot be easily separated. To address this issue, we will use the spectral representation of the kinetic energy.

The main goal of this paper is to present a method to conduct a selective damping of kinetic energy in the atomistic region. Digital filters will be used to remove the frequencies not representable by the coarser model. In this article, we mainly focus on linear filters as they are simpler to implement than non-linear filters. More details about the use of non-linear filters in multiscale simulations are presented elsewhere [31]. Thus, we will first address what are suitable cutoff wave vectors to ensure a sustainable transmission of the large wavelengths from one model to the other. We will select a criterion based on the dispersion relations of the atomistic and continuum models. The naturally following question is how to perform the selective damping. Our approach will be based on the generalized Langevin dynamics using a specified kernel function built with numerical filtering techniques commonly used in signal processing. This approach is described in earlier works [32–34] and was already used by other authors [35,36,29] in a coupling method with filtering acting on time oscillations. The innovation that we propose here uses spatial filtering acting on spatial oscillations, which we will demonstrate to be more efficient and easier to implement.

In the next section, we give a brief introduction to general digital filters. A discussion about the spectral decomposition of energy followed by the method to select a cutoff wavelength appropriate to coupling approaches is presented in the Sections 3 and 4. Then, we introduce a 1D numerical model – which is based on the generalized Langevin equation – as a tool for studying selective damping in Section 5. In Section 6, we present parametric studies based on time and spatial filtering. The criterion to compute the minimum filter size is presented. We also discuss the computation of the bridging zone size required in FE-MD coupling through an example. Finally, we validate our approach in two dimensional space with two examples in Section 7. In the conclusion, we summarize the important details required to perform spatial filtering.

2. Digital filters background

A digital filter is a mathematical operator acting on a sampled signal. It aims at reducing or enhancing certain frequencies of an input signal [37]. The filtering operation can be defined as the convolution in real space of a kernel function f of size F_S and an input signal $x(t)$ leading to an output signal $y(t)$. For continuous signals, it is given by the following equation:

$$y(t) = \int_{t-F_S}^{t} f(t-\tau)x(\tau)d\tau \tag{2.1a}$$

Based on the convolution theorem, the filtering can also be achieved in the frequency space given by [38]:

$$\hat{y}(\omega) = \hat{f}(\omega)\hat{x}(\omega) \tag{2.1b}$$

where $\hat{f}(\omega)$, $\hat{x}(\omega)$ and $\hat{y}(\omega)$ are the corresponding Fourier transforms of $f(t)$, $x(t)$ and $y(t)$ respectively.

The filtering operation presented by the Eq. (2.1a) is conducted in the time domain and mostly used in the electrical engineering and signal processing fields [37]. However, it can also be defined in the spatial domain as used in image processing [39]. Thus, the units of filter size F_S will change depending on the filtering domain (time or spatial). Moreover, as we deal mostly with discrete signals, it is worth presenting here the discrete form of convolution used in the remainder of the paper:

$$y(t) = \sum_{t-F_S}^{t} f(t-\tau)x(\tau) \tag{2.2}$$

As an example, when a modulated signal of frequencies 8 Hz and 100 Hz is filtered using a low or a high pass filter, we can obtain the low (resp. high) frequency component for a low (resp. high) pass filter as shown in Fig. 1(b). These low/high pass filters, presented in Fig. 1(a), are conveniently defined in the frequency space. Indeed, it is classical to define ideal pass band filters in the frequency space and perform an inverse Fourier transform to generate real space kernel functions f described by a set of real value coefficients. However, in order to maintain the ideal behavior, the size F_S of the generated filters f needs to be infinite. To generate finite size filters, windowing techniques can be used [37].

We used the Hanning window technique [38] to generate filters of a selected size F_S with a smooth transition from pass to stop band. For instance, a symmetrical low pass filter of size $F_S = 100\Delta t$ with a normalized (using Δt) cutoff frequency $v_{cut} = 0.05$ as well as its Fourier response for a range of frequencies, are shown in Fig. 2(a) and (b). Note that Δt is the timestep. The Fourier response or filter response is defined as the ratio of the filtered or output amplitude to its input amplitude, plotted with respect to frequency or wavelength. The response of the low pass symmetrical filter transmits, as expected, frequencies below the cutoff frequency. But, it is important to note that the filtered signals will have a delay in response equal to the size of the kernel function f. This is due to the shape of the kernel function f which is shifted from the time origin [38].

In order to remove the constraint of the delayed response, non-symmetrical filters can be used. For instance, a non-symmetrical low pass filter of size $F_S = 100\Delta t$ with a normalized cutoff frequency $v_{cut} = 0.05$ is shown in Fig. 3(a). Though a non-symmetrical filter does not have any time delay, its response is of very poor quality as shown in Fig. 3(b). This is expected as the half-kernel function f (non symmetrical filter) does not have the exact frequency definition of the perfect pass band filter due to the truncation.

3. Spectral energy decomposition

Any solid is an interacting set of atoms. The classical statistical physics approach leads to oscillatory models for which the dynamics is a superposition of waves of various amplitude and frequency. In this context, heat energy is defined as the kinetic energy of all waves making impossible, by definition, the separation of heat energy from mechanical energy. Nevertheless, for a macroscopic object at thermal equilibrium, large wavelengths are not present leaving only thermal noise contributing to kinetic energy. The relative contribution of each wave contributing to the dynamics is called the spectral distribution/decomposition and will be described further below.

The spectral decomposition of energy is the amount of energy per unit frequency or per unit wave vector [40]. This decomposition can be expressed with respect to wave vector or frequency