

A coarse-grained molecular dynamics model for crystalline solids

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SUMMARY

A general mathematical framework for coarse-graining molecular dynamics (MD) model for solid system is presented. The formulation is based directly on the full MD model. The reduction of the atomic degrees of freedom is accomplished using the Mori–Zwanzig projection method. We also demonstrate how to simplify the model under this framework to make the numerical implementation much easier. Copyright © 2010 John Wiley & Sons, Ltd.

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1. INTRODUCTION

Molecular dynamics (MD) models have been playing an increasingly important role in the study of material properties and behavior. A typical simulation requires to simulate a large number of atoms, making the computation extremely expensive. The chaotic nature of these systems further complicates the problem. In many practical situations, the behavior of interest occurs in a very localized region, e.g. near material defects, whereas the rest of the atoms merely act as the surrounding environment. Therefore, it is of considerable practical interest to develop an effective model in which the excessive atomic degrees of freedom is incorporated implicitly.

One model reduction approach is to combine the atomistic model directly with coarser descriptions, e.g. conventional continuum elasto-dynamics models. There has been a growing recent interest in developing such coupled methods, e.g. see [1–8]. The idea is to retain the full atomistic model near defects where the deformation is large, and away from defects, a continuum model is employed. The hope is to obtain an accuracy comparable to the full atomistic model, and an efficiency comparable to the pure continuum approach.

Despite the enormous success of these coupling approach, many fundamental questions still remain. For instance, how does the atomistic model ultimately give rise to the classical continuum equations? In addition, are there intermediate scales that the aforementioned methods fail to

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capture? Such a question calls for a more first-principle-based approach. The present paper is an attempt toward this direction. The proposed approach is directly based on the full atomistic model, without introducing any continuum model at the beginning. In the first step, we choose a set of coarse-grain (CG) variables that are representative of the overall dynamics. We then use a dimension reduction technique to derive the *exact* equations for the CG variables. Unfortunately, these equations are usually very difficult to implement numerically. Therefore, a crucial step is taken to simplify the CG equations to a form that is more computationally amenable.

The CG model derived here is similar to the CGMD model developed in [9, 10]. Their formulation employs a finite element representation, and the dimension reduction is done in the partition function by integrating out the excess atomic degrees of freedom. Therefore, the CG is based on the free energy. In this paper, we will show that CGMD model also arises in our formulation. However, the CG model derived directly from the equations of motion also contain history-dependent and random noise terms. They are not included in the CGMD model [9, 10].

Our approach is based on the Mori–Zwanzig formalism [11, 12], an elegant formulation for deriving the effective equation for pre-selected dynamic variables. The reduction procedure was later studied by Berne and Berne and Pecora in [13], and Chorin *et al.* in their work of optimal prediction [14, 15]. The advantage of this formulation is that (1) it is exact; (2) it separates out different contributions to the dynamics of the CG variables. However, the resulting equations are usually too complicated to implement numerically. On the other hand, for some special cases, e.g. when the atomic interaction is linear, these equations are greatly simplified. Examples include the well-known Zwanzig–Kac model of harmonic oscillators [16], the CG model proposed by Izvekov and Voth [17], and the defect model by Munakata [18]. However, in these works the atomic interaction is often assumed to be linear for all atoms, which is not accurate enough to describe geometric defects in solids. To balance the accuracy and the applicability of the CG model, we will show a modified harmonic approximation in which the atomic interaction near defects is fully retained, whereas away from defects, the usual harmonic approximation is applied. In addition to the more accurate harmonic approximation, the current formalism also allows flexible selection of the CG variables. Furthermore, it takes into account a pre-existing elastic field, which was not considered in the previous works.

In the case when the CG variables are all selected as atoms near defects, our projection procedure gives rise to the boundary condition for the computational domain consisting of the selected atoms. This case has been extensively studied [5, 6, 19–24]. This paper considers a more general case where the CG variables can be selected in the far field.

This paper is organized as follows. In Section 2, we discuss the Mori–Zwanzig formulation applied to MD, deriving an exact equation for a set of pre-selected CG variables. Then a simplified model is derived in Section 3. We will study the energy balance in Section 4. Finally, we present an one-dimensional example in Section 5.

2. THE MATHEMATICAL FORMULATION

We consider the MD model.

$$m\ddot{\mathbf{u}}_i = -\nabla_{\mathbf{u}_i} V. \quad (1)$$

Here we have chosen the displacement, denoted by \mathbf{u}_i , to describe the motion of the atoms; $V(\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_N)$ is the interatomic potential; N is the total number of atoms.

The first step in the CG procedure is to pick the CG variables. Let \mathbf{u} and \mathbf{v} be, respectively, the displacement and the velocity of all the atoms in the system. We choose the CG variables as follows:

$$\mathbf{q} = B\mathbf{u}, \quad \mathbf{p} = mB\mathbf{v}, \quad (2)$$

where B is an $n \times N$ matrix with rank dn , with d being the dimension. In practice, B can be chosen, for instance, as a subset of atoms, which are similar to the representative atoms in the quasicontinuum method [25–27]. One may also choose B so that \mathbf{q} corresponds to the local average of a cluster of atoms, or to the nodal values of a finite element method [9, 10]. In these cases, one expects that as one approaches to continuum scale, the CG models are reduced to a finite volume or a finite element model. The flexibility of choosing the CG variables is a main advantage of this current approach.

To apply the Mori–Zwanzig formalism, it is convenient to define the Liouville operator as follows:

$$\mathcal{L} = \mathbf{v} \cdot \nabla_{\mathbf{u}} - \frac{1}{m} \nabla V \cdot \nabla_{\mathbf{v}}. \quad (3)$$

For any dynamic variable A , we can write, $A(t) = e^{tL} A(0)$. Let \mathcal{P} be a projection operator on functions of \mathbf{u} and \mathbf{v} . It will be specified in the next section. Once the dynamic variables and the projection are defined, the Mori–Zwanzig procedure yields [11–15]

$$\frac{d}{dt} A(t) = e^{t\mathcal{L}} \mathcal{P} \mathcal{L} A(0) + \int_0^t e^{(t-s)\mathcal{L}} K(s) ds + F(t), \quad (4)$$

where

$$F(t) = e^{t\mathcal{L}} \mathcal{Q} \mathcal{L} A(0), \quad K(t) = \mathcal{P} \mathcal{L} F(t). \quad (5)$$

The first and the second terms on the right-hand side depend only on the CG variables. They represent, respectively, the Markovian contribution and the history dependence of the dynamics. The third term, which satisfies $\mathcal{P}F = 0$, is unresolved and typically regarded as random noise.

In our formulation, the projection operator is defined as the conditional expectation given the CG variables,

$$\mathcal{P} = E[\cdot | (\mathbf{q}, \mathbf{p})]. \quad (6)$$

3. SIMPLIFIED MORI–ZWANZIG MODEL

Although in principle the conditional average can be defined with respect to the Gibbs distribution, it is usually difficult to compute due to the large dimension of the entire system. In addition, the resulting MZ model is often too complicated to implement. Therefore, we will introduce an approximation to simplify the MZ model. We start by seeking the mechanical equilibrium of the system. This is found by minimizing the potential energy while keeping the CG variables fixed. With a harmonic approximation, the displacement at the mechanical equilibrium is given by

$$\mathbf{u} = R\mathbf{q}, \quad R = D^{-1} B^T (B D^{-1} B^T)^{-1}, \quad (7)$$

where D is the force constant at the reference state. The derivation is given in the appendix. The matrix R reconstructs the displacement field. In particular, the matrix P_u , $P_u = RB$, defines a projection to the space spanned by the CG variable \mathbf{q} . It also appeared in the CG model [9, 10]. We let Q_u be the corresponding complementary projection,

$$Q_u = I - P_u. \quad (8)$$

Equation (7) was derived assuming that there is no external force applied. If an external force, \mathbf{f}^{ex} , is present, one finds that

$$\mathbf{u} = \Phi(q) = R\mathbf{q} + Q_u D^{-1} \mathbf{f}^{\text{ex}}. \quad (9)$$

The equation above defines an approximate equilibrium state for the remaining degrees of freedom. A Taylor expansion around this mechanical equilibrium yields the following approximation of the total Hamiltonian:

$$H(\mathbf{u}, \mathbf{v}) \approx \frac{m\mathbf{v}^2}{2} + V(P_u \mathbf{u}) + \frac{1}{2} \mathbf{u}^T Q_u^T D Q_u \mathbf{u}. \quad (10)$$

The terms with first-order gradient dropped out since the expansion is about a mechanical equilibrium.

This approximation will be applied to both the equations of motion, to be derived from the Hamilton's principle, and the conditional expectation. More specifically, Equation (1) becomes

$$m\ddot{\mathbf{u}} = -P_u^T \nabla V(P_u \mathbf{u}) - Q_u^T D Q_u \mathbf{u}. \quad (11)$$

Meanwhile the initial state of the system and the projection operator are defined according to probability density,

$$\rho(\mathbf{u}, \mathbf{v}) = \frac{1}{Z} \int e^{-\beta[V(P_u \mathbf{u}) + (1/2)(\mathbf{u} - \bar{\mathbf{u}})^T D (\mathbf{u} - \bar{\mathbf{u}}) + (m/2)(\mathbf{v} - \bar{\mathbf{v}})^2]} d\mathbf{u} d\mathbf{v}. \quad (12)$$

Notice that we have introduced some mean values $\bar{\mathbf{u}}$ and $\bar{\mathbf{v}}$. This is necessary when an existing displacement and velocity field is present initially.

In this case, the projection operator, when applied to a linear function, corresponds to a matrix multiplication. More specifically, we have

$$\mathcal{P}\mathbf{u} = \bar{\mathbf{u}} + P_u(\mathbf{u} - \bar{\mathbf{u}}), \quad \mathcal{P}\mathbf{v} = \bar{\mathbf{v}} + P_v(\mathbf{v} - \bar{\mathbf{v}}), \quad (13)$$

where $P_v = B^T(BB^T)^{-1}B$. In the matrices P_u and P_v , the matrix inverse is well defined because B has full rank.

The following properties of these projection matrices can be easily verified:

$$Q_v^T = Q_v, \quad Q_v B^T = 0, \quad (14a)$$

$$Q_u D^{-1} B^T = 0, \quad D Q_u = Q_u^T D, \quad (14b)$$

$$B Q_u = 0, \quad Q_u Q_v = Q_v. \quad (14c)$$

We now follow the MZ procedure to derive the effective equations for \mathbf{q} and \mathbf{p} . First, we notice that $\dot{\mathbf{q}} = \mathbf{p}/m$. In the following calculation, we choose $A = \mathbf{p}$ in (4).

3.1. The Markovian term

The first term on the right-hand side of Equation (4) is usually written as a mean force. The corresponding free energy is given by

$$\mathcal{F}(\mathbf{q}, T) = -k_B T \log \int e^{-\beta V} \delta(\mathbf{u} - B\mathbf{q}) d\mathbf{u}.$$

Then the first term is given by

$$e^{t\mathcal{L}} \mathcal{P} \mathcal{L} \mathbf{p}(0) = -\langle \nabla_{\mathbf{q}} \mathcal{F} \rangle.$$

The average is with respect to the usual canonical distribution.

With the harmonic approximation, the mean force is reduced to

$$e^{t\mathcal{L}} \mathcal{P} \mathcal{L} \mathbf{p}(0) = -BP_u^T \nabla V(R\mathbf{q}) - BDQ_u \bar{\mathbf{u}}. \quad (15)$$

3.2. The random noise

We now compute the random force. Notice that

$$F(0) = \mathcal{L} \mathbf{p}(0) = -BDQ_u(\mathbf{u}(0) - \bar{\mathbf{u}}),$$

and in light of (14c),

$$\dot{F}(0) = \mathcal{L} F(0) = -BDQ_v(\mathbf{v}(0) - \bar{\mathbf{v}}).$$

Repeating these calculations one sees that the random force can be written in the form of

$$F(t) = C(t)(\mathbf{u}(0) - \bar{\mathbf{u}}) + S(t)(\mathbf{v}(0) - \bar{\mathbf{v}}). \quad (16)$$

The coefficients $C(t)$ and $S(t)$, which are $n \times N$ matrices, are defined below. The calculation also suggests that the initial condition be given by

$$C(0) = -BDQ_u, \quad S(0) = 0. \quad (17)$$

Next with direct calculations one gets

$$\begin{aligned} \mathcal{L} F &= C(t)\mathbf{v}(0) - S(t)D\mathbf{u}(0)/m, \\ \mathcal{L} \mathcal{L} F &= C(t)Q_v(\mathbf{v}(0) - \bar{\mathbf{v}}) - S(t)DQ_u(\mathbf{u}(0) - \bar{\mathbf{u}})/m. \end{aligned} \quad (18)$$

Meanwhile from (5), one must have that $\dot{F} = \mathcal{L} F$, which would be satisfied if $C(t)$ and $S(t)$ are solutions of the equations

$$\begin{aligned} m\dot{C} &= -S(t)DQ_u, \\ \dot{S} &= C(t)Q_v. \end{aligned} \quad (19)$$

In particular, using the properties (14a)–(14c), we find that $C(t)$ and $S(t)$ solve the equations

$$\begin{aligned} m\ddot{C}(t) &= -C(t)Q_v D, \quad C(0) = -BDQ_u, \quad \dot{C}(0) = 0, \\ m\ddot{S}(t) &= -S(t)DQ_v, \quad S(0) = 0, \quad \dot{S}(0) = -BDQ_v. \end{aligned} \quad (20)$$

It follows from these equations that the orthogonality condition, $\mathcal{P}F=0$, in the MZ formulation holds. In particular, we have

$$C(t)Q_u = C(t), \quad S(t) = S(t)Q_v. \quad (21)$$

Therefore, the equation for $S(t)$ can be written in a symmetric form

$$m\ddot{S}(t) = -S(t)Q_v D Q_v. \quad (22)$$

We now compute the correlation of $F(t)$. Clearly, it is a Gaussian process with zero mean. In the light of the initial condition (17), the time correlation is

$$\langle F(t+t_0)F(t_0)^T \rangle = k_B T \theta(t), \quad (23)$$

where

$$\theta(t) = -C(t)B^T. \quad (24)$$

This shows that $F(t)$ is a stationary process.

3.3. The memory term

We now proceed to compute the memory term. From (5) and (18), we have

$$K(t) = C(t)P_v \mathbf{v}(0) + C(t)Q_v \bar{\mathbf{v}} - S(t)DQ_u \bar{\mathbf{u}}. \quad (25)$$

Here we have dropped the term $S(t)DP_u \mathbf{u}(0)$, which vanishes owing to (14c) and (21). It follows from (5), (19), (20) and (24) that

$$\int_0^t e^{(t-s)\mathcal{L}} K(s) ds = - \int_0^t \theta(t)(BB^T)^{-1} \mathbf{p}(t-s) ds + C(t)\bar{\mathbf{u}} + S(t)\bar{\mathbf{v}} + BDQ_u \bar{\mathbf{u}}.$$

Finally we define the mass matrix $M = m(BB^T)^{-1}$, $G(t) = (BB^T)^{-1}F(t)$, and the MZ equation reads

$$\begin{aligned} \dot{\mathbf{q}} &= \mathbf{p}/m, \\ M\dot{\mathbf{p}} &= -R^T \nabla V(R\mathbf{q}) - \int_0^t \Theta(\tau) \mathbf{p}(t-\tau) d\tau + G(t) + \mathbf{f}_0, \end{aligned} \quad (26)$$

where

$$\Theta(t) = (BB^T)^{-1} \theta(t) (BB^T)^{-1} \quad (27)$$

is a memory kernel, and

$$\mathbf{f}_0(t) = C(t)\bar{\mathbf{u}} + S(t)\bar{\mathbf{v}}$$

comes from the preexisting elastic field.

This is a generalized Langevin equation (GLE). In particular, the fluctuation-dissipation theorem [28] holds:

$$\langle G(t+t_0)G(t_0)^T \rangle = k_B T \Theta(t). \quad (28)$$

The memory kernel can be expressed explicitly by combining Equations (20), (22), (24) and (27):

$$\theta(t) = BQ_u^T DQ_u B^T - \frac{t^2}{m} BDQ_v \Phi(t\Omega) Q_u B^T. \quad (29)$$

Here $\Omega = \sqrt{Q_v D Q_v}$, and $\Phi(\omega) = (1 - \cos(\omega))/\omega^2$, with an extension to matrix-valued function by the Taylor series.

Notice that the memory kernel only depends on the matrices B and D . It is independent of the temperature, a crucial difference between the current model and some of the previous CG models. This is another advantage of using conditional expectation as the projection operator.

4. ENERGY DISSIPATION

Here we demonstrate that in general, the GLE is an irreversible process. Let us assume that $k_B T = 0$, i.e. the temperature is zero, and so $G(t) = 0$. In addition, we assume that

$$\bar{\mathbf{u}} = \text{range}(D^{-1} B^T) \quad \text{and} \quad \bar{\mathbf{v}} = \text{range}(B^T). \quad (30)$$

From (14a) and (14b), we find that $\mathbf{f}_0(t) = 0$. We define the energy of the system as

$$E(t) = V(R\mathbf{q}) + \frac{1}{2} \mathbf{p}^T M^{-1} \mathbf{p}. \quad (31)$$

Then we have the energy balance

$$\dot{E}(t) = -J, \quad J = \mathbf{p}^T \int_0^t \Theta(\tau) \mathbf{p}(t - \tau) d\tau. \quad (32)$$

Using the fact that the power spectrum, the Fourier transform of the correlation matrix $\Theta(t)$, is semi-positive-definite, one can show that [29]

$$\int_0^t J(\tau) d\tau \geq 0, \quad (33)$$

for any $t \geq 0$. As a result,

$$E(t) \leq E(0).$$

5. A ONE-DIMENSIONAL EXAMPLE

From Equations (26) and (28), we see that the memory kernel determines both the history-dependent term and the random noise. Once the memory function is available, the GLE (26) can be solved numerically. Next, we investigate the kernels for different choices of the CG variables. For demonstration purpose, we consider a one-dimensional chain model, in which the equation of motion is given by

$$m\ddot{u}_i = \varphi'(u_{i+1} - u_i) - \varphi'(u_i - u_{i-1}). \quad (34)$$

Here the function φ models the pairwise interaction, e.g. the Lennard–Jones potential.

For this model, the force constants are $D_0 = -2\phi''(0)$ and $D_{\pm 1} = \phi''(0)$. To define the CG variables, we divide the system into a number of cells of the same width, and three models are considered where the CG variables are selected as the displacement and velocity of

- (1) one atom out of K atoms in each cell;
- (2) the average of every K atoms in each cell;
- (3) the nodal values of a linear finite element model defined at the cell interfaces. In this case, B^T corresponds to an interpolation from the CG variables to all the atoms.

For all the three cases, the length of the chain is chosen long enough to model a large system, and we expect that diagonal entries of the kernel are the same for all blocks. In the numerical experiments, the memory kernels for various values of K are plotted in Figure 1. We found that all three models will approach to a continuum limit, i.e. the limiting model as K goes to infinity. For case (1), we find that as one increases K , the kernel function converge, and the limiting function can be identified as a Bessel function, $J_1(2t)/t$. This kernel function has been found in the GLE model in [30, 31], where it was derived as an interface condition at a gas–solid surface. For cases (2) and (3), the kernel function diminishes for large K . We have found an asymptotic behavior of K^{-1} and K^{-2} for the correlation function at $t=0$. See Figure 2. But these trends do not continue: when a quadratic finite element is used to define the CG variables, the decay rate of the kernel is still K^{-2} .

For selection schemes (2) and (3), if the initial condition can already be well approximated by a finite volume or a finite element representation, then one can choose $\tilde{\mathbf{u}} = \tilde{\mathbf{v}} = 0$. For section scheme (1), however, they have to be specified explicitly in practice.

6. CONCLUSION AND DISCUSSIONS

We have presented mathematical framework for deriving CG models based on the full molecular dynamics model. The main ingredients are: (1) choosing the CG variables as linear functions of the atom displacement and momentum; (2) linearizing the atomic interaction for the remaining degrees of freedom around an approximate equilibrium state. The main advantage of the CG model is the flexibility to choose the CG variables, and the nice structure of the random noise: with the fluctuation-dissipation theorem, the noise can be sampled from the kernel function. As a result, some of the implementation issues associated with the MZ formalism is avoided.

A one-dimensional problem was considered as an example. In principle, the formulation applies to two- and three-dimensional cases. However, to fully carry out this program, several issues need to be further addressed: The first issue is the calculation of the mean force. The current approximation reduces the mean force to a rather simple form. The problem is that the formula involves ∇V , the force on every atom. This is not practical, especially in regions where the cells are large. For model (1), this can be simplified considerably because the matrix B selects a small subset of atoms. Since most interatomic potentials have a cut-off radius, only the close neighbors of the selected atoms need to be visited. For models (2) and (3), recall that the operator R reconstructs the atom displacement from the CG variables. If the displacement field is smooth away from local defects, certain approximations, such as a quadrature formula can be used. In addition, the dependence of the mean force on the temperature is not present in the harmonic approximation. To improve the accuracy, a reweighing technique for free energy calculation may be needed.

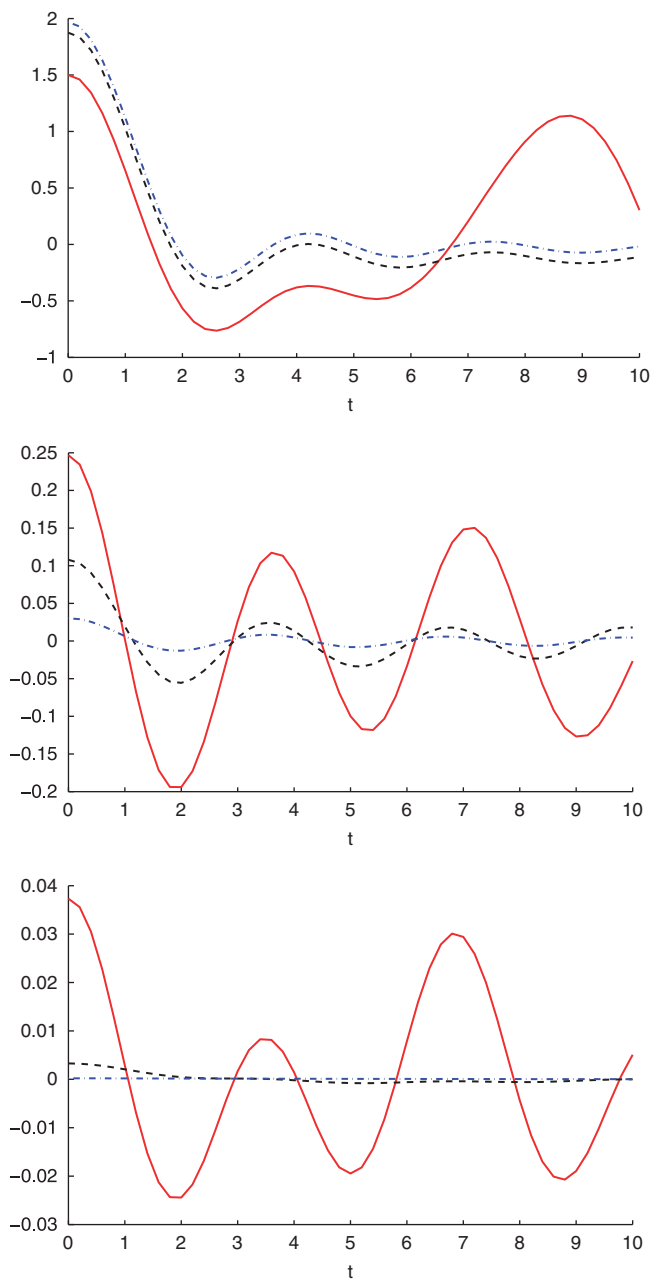


Figure 1. Memory kernels for the one-dimensional chain model. From top to bottom, the CG models (1)–(3). Solid lines: $K = 4$; dashed lines: $K = 32$; dashed-dot lines: $K = 128$. In the middle figure, we also plotted the kernel at $t = 0$ for various values of K .

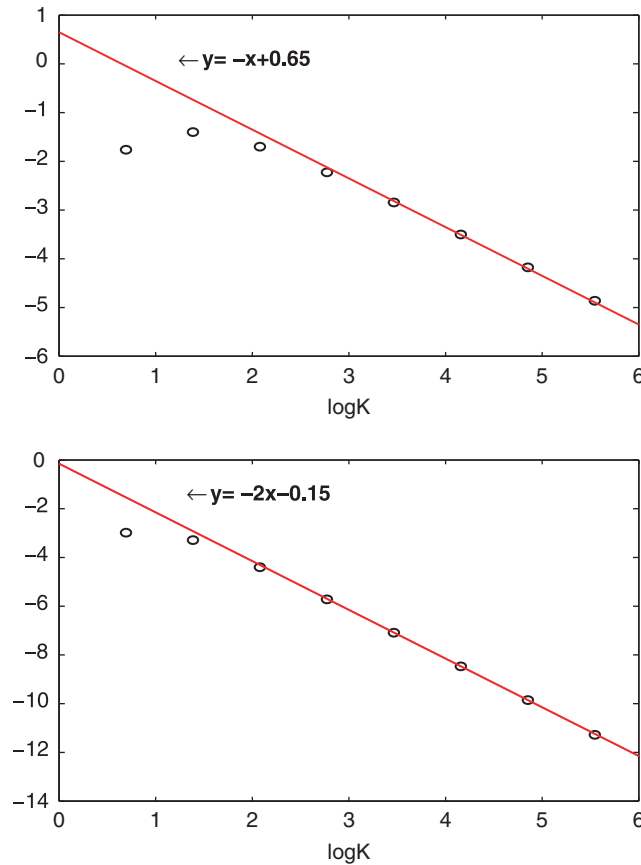


Figure 2. Memory kernels for the one-dimensional chain model at time $t=0$. From top to bottom, the CG models (2)–(3). Circles: the values of $\theta(0)(BB^T)^{-1}$ are plotted for several values of K on a log-log scale; solid lines: the linear fitting functions.

The second issue is the computation of R and the memory kernel. In principle, it can be computed from Equations (7) and (27). However, it is not feasible computationally since the dimension of the matrices are quite large. In the context of boundary conditions, they can be found via alternative means, e.g. from lattice Green's functions or from a variational approach based on the phonon spectrum [21–23, 32] for three-dimensional systems. We expect that the same techniques can be applied here. Another observation is that the memory terms do not appear in the core regions where all the atoms are chosen. In addition, when local averages or finite element nodal values are selected as CG variables, the memory terms are diminishing as one approaches to large scales. Therefore, it is only necessary to compute these kernel functions in the transition regions. Once the kernel is found, the random noise term can be computed from the fluctuation-dissipation theorem.

The third issue is how to compute the force \mathbf{f}_0 . This problem has been studied in the context of boundary conditions [22], in which the atomistic system is surrounded by an elastic medium. The idea is that since $\bar{\mathbf{u}}$ and $\bar{\mathbf{v}}$ can be assumed to be smooth, they can be replaced by a continuum

model, which is similar to linear elasto-dynamics. For models (2) and (3), it is possible to show that \mathbf{f}_0 is small if $\bar{\mathbf{u}}$ and $\bar{\mathbf{v}}$ correspond to smooth continuous functions. These issues will be discussed in separate works.

APPENDIX A

Here, we compute an approximate solution to the displacement at the mechanical equilibrium. It is the solution of

$$\min V(\mathbf{u}) \quad \text{subject to } B\mathbf{u} = \mathbf{q}.$$

Let C be an $(N-n)$ -by- n matrix, defining the remaining degrees of freedom $\tilde{\mathbf{u}}$, $\tilde{\mathbf{u}} = C\mathbf{u}$. The final form of the displacement will be independent of the choice of B . The matrix

$$\begin{bmatrix} B \\ C \end{bmatrix}$$

is assumed to be invertible, and its inverse is given by $[\Sigma_1 \ \Sigma_2]$, which has been partitioned accordingly. The total displacement is then given by $\mathbf{u} = \Sigma_1 \mathbf{q} + \Sigma_2 \tilde{\mathbf{u}}$. Minimizing the potential energy with respect to $\tilde{\mathbf{u}}$, we get $\Sigma_2^T \nabla V = 0$, and with the harmonic approximation, it becomes

$$\Sigma_2^T D \Sigma_1 \mathbf{q} + \Sigma_2^T D \Sigma_2 \tilde{\mathbf{u}} = 0.$$

Solving $\tilde{\mathbf{u}}$ yields the displacement at the mechanical equilibrium

$$\mathbf{u} = (\Sigma_1 - \Sigma_2 (\Sigma_2^T D \Sigma_2)^{-1} \Sigma_2^T D \Sigma_1) \mathbf{q}. \quad (\text{A1})$$

We now show that the matrix on the right-hand side corresponds to the projection matrix P_u . Notice that

$$\left(\begin{bmatrix} B \\ C \end{bmatrix} D^{-1} \begin{bmatrix} B^T & C^T \end{bmatrix} \right)^{-1} = \begin{bmatrix} \Sigma_1^T \\ \Sigma_2^T \end{bmatrix} D \begin{bmatrix} \Sigma_1 & \Sigma_2 \end{bmatrix}.$$

Using the blockwise matrix inversion formula, we find that

$$\Sigma_1^T D \Sigma_1 - \Sigma_1^T D \Sigma_2 (\Sigma_2^T D \Sigma_2)^{-1} \Sigma_2^T D \Sigma_1 = (B D^{-1} B^T)^{-1}.$$

Left multiplying the equation by $D^{-1} B^T$, and using $B^T \Sigma_1^T = I - C^T \Sigma_2^T$, we get

$$\Sigma_1 - \Sigma_2 (\Sigma_2^T D \Sigma_2)^{-1} \Sigma_2^T D \Sigma_1 = D^{-1} B^T (B D^{-1} B^T)^{-1}.$$

This completes the proof.

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