Journal of Computational Physics 343 (2017) 110–114

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Short note

Time- and memory-efficient representation of complex mesoscale potentials

Grigory Drozdov, Igor Ostanin *, Ivan Oseledets

ARTICLE INFO

Article history:
Received 14 July 2016
Received in revised form 19 April 2017
Accepted 21 April 2017
Available online 28 April 2017

Keywords:
Mesoscale modeling
Tensor train cross approximation

ABSTRACT

We apply the modern technique of approximation of multivariate functions – tensor train cross approximation – to the problem of the description of physical interactions between complex-shaped bodies in a context of computational nanomechanics. In this note we showcase one particular example – van der Waals interactions between two cylindrical bodies – relevant to modeling of carbon nanotube systems. The potential is viewed as a tensor (multidimensional table) which is represented in compact form with the help of tensor train decomposition. The described approach offers a universal solution for the description of van der Waals interactions between complex-shaped nanostructures and can be used within the framework of such systems of mesoscale modeling as recently emerged mesoscopic distinct element method (MDEM).

Introduction

Mesoscale coarse-grained mechanical modeling [1–4] is an important tool for *in silico* characterization of nanostructures. The typical coarse-grained modeling approach is based on the idea of the representation of a nanostructure (*e.g.* nanotube, nanoparticle, *etc.*) as a set of elements, which are treated either as point masses or solid bodies (rigid or deformable), interacting via bonding or non-bonding potentials. Compared to regular molecular dynamic (MD) approaches, such models are easily as scalable as MD, while rendering much higher computational efficiency. For example, they can be used for accurate mechanical modeling of the representative volume elements of complex nanostructured materials. However, such models require the efficient and reliable description of van der Waals (vdW) interaction potentials between complex-shaped elements. Such potentials depend on multiple parameters. For example, the interaction between two rigid bodies of a fixed size requires tabulation of six-dimensional array with good precision. The description of interactions between the bodies of variable size, which is required for adaptive models, or interactions between deformable elements, requires even more degrees of freedom and leads to larger multidimensional arrays of data. This makes simple tabulation of such potentials impractical, since the time to construct such a table and the memory to store it grows exponentially with the number of dimensions (the problem known as “curse of dimensionality”). The approach that is often used in the field is to design relatively simple analytical approximations for such interaction potentials, representing the potentials sought as separable functions [2,3]. Such an approach may be efficient in some situations, but in many cases it leads to over-simplifications and incorrect mechanics on the larger scale. In this work we suggest the reliable and universal approach for storing arbitrarily complex mesoscale potentials as compressed multidimensional tables (following the terminology accepted in data science and computational linear algebra communities, such tables will be referred to as tensors below). The compression is reached

* Corresponding author.
E-mail address: i.ostanin@skoltech.ru (I. Ostanin).

http://dx.doi.org/10.1016/j.jcp.2017.04.056
0021-9991/

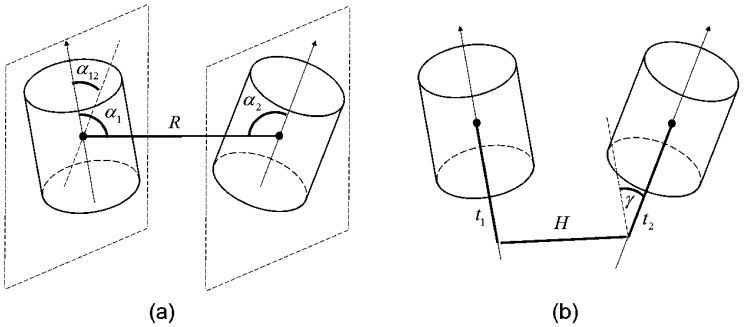

Fig. 1. Two possible parameterizations of mutual position of two cylinders.

via tensor-train cross approximation [5,6]. It allows to construct the approximation of a tensor with the desired precision, using relatively small number of explicitly computed potential values. Such approaches were applied earlier in the field of computational chemistry [7], however, they are still widely unknown to the community of multiscale mechanical modeling. In order to demonstrate the pipeline of tensor approximation in application to mesoscale models, we consider relatively simple yet practically important problem of the vdW interaction between two equal-sized cylinders. This problem is important in a context of mesoscale mechanical modeling of large assemblies of carbon nanotubes (CNTs). As has been showed earlier, the use of simple pair potentials for the description of intertube interactions between cylindrical CNT segments leads to significant artifacts in model's behavior. In the previous works [2,3] the problem was addressed with sophisticated analytical approximations. However, these approximations can not be transparently generalized onto more complex situations – CNTs of different diameters, curved CNT segments *etc.* Our approach presented here does not suffer from such a lack of generality and can be used in a number of similar problems of the description of interactions between complex-shaped nanostructures.

Method

In this section we describe our technique of construction of the compressed table of the interaction potential between complex-shaped bodies with the example of vdW interactions between two equal-sized cylindrical segments of CNTs. Following the coarse-graining approach developed in [3,4], we idealize CNT segments as interacting cylindrical surfaces of uniform density. Total vdW interaction between two segments is found via the integration of standard Lennard–Jones (LJ) potential:

$$u_{LJ}(r) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right) \tag{1}$$

where r is the distance between particles, $\sigma\sqrt[6]{2}$ is the equilibrium distance, $-\varepsilon$ is the energy at the equilibrium distance. For carbon–carbon interaction, we accept $\sigma = 3.851$ Å, $\varepsilon = 0.004$ eV. In order to avoid the integration of an artificial singular part of LJ potential, we replace the potential in near-singular region $(0, r_0), r_0 = 3.8$ Å, with the cubic spline $u(r)$, satisfying $u(0) = 3$ eV, $u'(0) = 0, u(r_0) = u_{LJ}(r_0), u'(r_0) = u'_{LJ}(r_0)$.

We assume that carbon atoms are uniformly distributed over surfaces of cylinders with the surface density $\rho = \frac{4}{3\sqrt{3}a_{C-C}}$, where $a_{C-C} = 1.42$ Å is the equilibrium carbon–carbon bond length. The potential between cylindrical segments of nanotubes is then represented as the integral over the surface of each cylinder:

$$U_t = \int_{S_1}\int_{S_2} \rho^2 u_{LJ}(r)\, dS_1 dS_2 \tag{2}$$

where S_1 and S_2 are cylinders side surfaces, dS_1 and dS_2 are the elements of surfaces, r is the distance between dS_1 and dS_2. The shapes of function r for different parametrizations are given in the Appendix. In order to describe the mutual position and orientation of two cylinders one needs four independent variables – six variables for general rigid bodies are reduced by two due to axial symmetries of the cylinders. Since the choice and order of these four variables is important for the approximation technique we intend to use, we compare two different parameterizations. The first one includes one distance and three angles $(R, \alpha_1, \alpha_2, \alpha_{12}$ (Fig. 1(a))), whereas the second utilizes three distances and one angle $(t_1, t_2, H, \gamma$ (Fig. 1(b))). For both choices of independent variables, we specify the regular grid in four-dimensional space with the appropriate tabulation limits. We sample n points along each independent variable, which results in n^4 tabulated potential values.

Clearly, it is impossible to perform such expensive calculations "on the fly" for millions of interacting bodies. Therefore, within the direct approach we have to tabulate this potential function on multidimensional dense grid. It is possible for