Time- and memory-efficient representation of complex mesoscale potentials

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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 via tensor-train cross approximation [6,7]. 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 [8], 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 pratically 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 $(0, r_0), r_0 = 3.8 \text{Å}$, 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 $a_{C-C} = 1.42\text{Å}$ 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:

$$U_{t} = \int_{S_{1}} \int_{S_{2}} \rho^{2} u_{LJ}(r) dS_{1} dS_{2}$$
 (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 choise 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 ($t_1, t_2, H, \gamma(\text{Fig. 1(b)})$). 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.

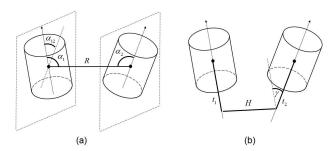


Figure 1: Two possible parameterizations of mutual position of two cylinders

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 our rather simple example, but becomes computationally prohibitive in terms of required time and memory for more complex structures and corresponding potentials. Below we describe a general approach that is capable to compute such multidimensional tables fast and store them in a compact form.

Our approach is based on tensor train decomposition (TT) and tensor train cross approximation [6, 7]. In the TT format each element of d-dimensional tensor $U(i_1, i_2, \ldots, i_d)$ is represented as the product of d matrices:

$$U(i_1, i_2, \dots, i_d) = \sum_{\alpha_0, \alpha_1, \dots, \alpha_d} G_1(\alpha_0, i_1, \alpha_1) G_2(\alpha_1, i_2, \alpha_2) \dots G_d(\alpha_{d-1}, i_d, \alpha_d)$$
(3)

Here indices α_k are changing from 1 to r_k , which are called TT-ranks. Each matrix G_k ($\alpha_k - 1, i_k, \alpha_k$) has the size $r_{k-1} \times r_k$, depends on only one index of the original tensor, and these matrices form the three-dimensional tensors, which are called cores of the TT-decomposition. r_0 and r_d are assigned to 1. Intermediate TT ranks r_k are determined by the TT approximation procedure to provide given approximation precision ϵ_{tt} and are conditioned by the structure of the approximated tensor.

Since tensors generated by the discretization of physically meaningful functions are typically ether low-rank or well approximated by the low-rank tensors, the decomposition (3) provides a powerful tool to represent such tensors in a compact form. The technique of construction of the best approximation in TT format with a given precision is described in [7]. In this work we use the standard package TT toolbox for construction of the low-rank approximation of our potential. In application to mesoscale modeling, TT decomposition can be used in two different ways. The first way is to accelerate the design of a full potential table and the second - to store it in a compact form. In the latter case the calculation of a single value of the potential in a nodal point would require computation of d matrix-vector products, with matrix dimensions $r_{k-1} \times r_k$.

Results and discussion

We constructed TT decompositions for a tensor of cylinder-cylinder interactions, for few different values of mesh refinement and accuracy. The potential of interaction between two cylindrical segments of (10,10) CNTs with the radius $R_c = 6.78\text{Å}$ and height $2R_c = 13.56\text{Å}$ was considered. The four-dimensional integral (2) was computed using regular rectangle quadratures over azimuthal angles of cylinders, and Gauss quadratures over cylinders axial directions. The number of integration points was chosen adaptively to provide the desired integration precision $\epsilon_i = 10^{-3}$. In order to keep our computations fast, we restricted ourselves with the best integration precision $\epsilon_i = 10^{-3}$. In our case of four-dimensional tensor TT-decomposition contains two matrices and two three-dimensional tensors as TT-cores. The tensor indices correspond to the sampling of the continuous potential function on a regular grid: $U(i_1,i_2,\ldots,i_d)=U_t(x_1,x_2,\ldots,x_d)$, where $x_d=x_d^{min}+i/n\cdot(x_d^{max}-x_d^{min})$. The tabulation limits (x_d^{min},x_d^{max}) for both parametrizations are given in Table 1.

We can define the compression of the tensor as the ratio of the numbers of elements in the initial tensor and in all the cores of the resulting TT-decomposition.

Table 1: Tabulation limits for two paremetrizations used.

Parametrization 1		Parametrization 2		
R	$(2R_c, 5R_c)$	H	$(2R_c, 5R_c)$	
α_1	$(0,\pi)$	t_1	$(-5R_c, 5R_c)$	
α_2	$(0,\pi)$	t_2	$(-5R_c, 5R_c)$	
α_{12}	$(0,\pi)$	γ	$(0,\pi)$	

The TT compression was performed for two different parameterizations of cylinders mutual position and different orders of variables (TT decomposition is not invariant with respect to permutation of tensor indices, our results are given for TT decompositions with the permutation of variables providing the lowest ranks of TT cores and the best compression). Tables 2 and 3 give the compression number obtained for the first and second parametrizations respectively, as a function of the grid refinement (number of points per each dimension) and the requested approximation precision ϵ_{tt} . It appears that even black-box application of the TT algorithm gives significant compression of the original tensor (which also roughly corresponds to the time needed to construct this tensor approximation).

Table 2: The compression for the first parameterization

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	TT approximation precision ϵ_{tt}						
		10^{-3}	10^{-2}				
\overline{n}	Max rank	Compression, %	Max rank	Compression, %			
10	20	29.4	13	18.2			
20	41	13.6	16	3.4			
30	47	5.3	16	1			
40	48	2.4	16	0.4			

Table 3: The compression for the second parameterization

	$\overline{\mathrm{TT}}$ approximation precision ϵ_{tt}					
		10^{-3}	10^{-2}			
\overline{n}	Max rank	Compression, %	Max rank	Compression, %		
10	27	44.8	19	30		
20	65	24.7	33	10.2		
30	85	12.1	38	3.4		
40	96	6.3	39	1.5		

Figure 2 illustrates the quality of the approximation of a complex potential relief at few cross-sections that correspond to in-plane (a) and out-of-plane (b) rotaton of one cylinder with respect to another for different intercenter distances. As we can see, the compressed potential representation fully reproduce original tensor.

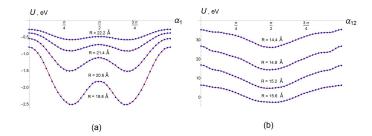


Figure 2: The potential in the first parametrization $(U(R, \alpha_1, \alpha_2, \alpha_{12}), \text{ solid red})$ and its TT approximation (dotted blue, n = 50, $\epsilon_{tt} = 10^{-2}$), as a function of one of parametrization angles and few different values of R: (a) $\alpha_1 \in (0, \pi)$, $\alpha_2 = 0$, $\alpha_{12} = 0$, R = 19.8, 20.6, 21.4, 22.2, (b) $\alpha_{12} \in (0, \pi)$, $\alpha_1 = 0$, $\alpha_2 = 0$, R = 14.4, 14.8, 15.2, 15.6.

Conclusion

In this note we have demonstrated the successful application of the technique that have recently emerged in the community of computational multilinear algebra - tensor-train cross approximation - to the problem of representation of the interaction potentials in modern mesoscale models. Within this approach the multidimensional potential table can be constructed based on just few direct calculations of the potential values, which dramatically accelerates construction of such a table. In the case when memory efficient representation is required, this table can be stored in a compact form and then each required value of the potential can be recovered at a moderate computational cost. In case when performance of on-the-fly computations is the highest priority, our approach can be used for fast construction of the full multidimensional table. The instruments for such approximation are freely available as components of the open source software TT-toolbox (https://github.com/oseledets/ttpy), and our code, performing the approximation of cylinder-cylinder vdW interaction potential, can be found at https://bitbucket.org/iostanin/cnt_potential_tt_compression/. The resulting approximations can be easily stored in either full or compact form, and further used in the framework of such existing mesoscale models as MDEM [3–5]. Our approach appears to be particularly useful for the problems involving interactions between complex deformable shapes - e.g. CNT segments with variable length, radius, curvature and flatness.

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Appendix

Here we give the explicit shapes for the functions r for two parameterizations used. In both cases the distance depends on four variables describing the mutual position of two cylinders, and four more variables - axial coordinates z_1, z_2 and azimuthal angles φ_1, φ_2 , describing the positions of surface elements dS_1 and dS_2 on cylinders' side surfaces. First parameterization:

$$r(dS_1, dS_2) = r(R, \alpha_1, \alpha_2, \alpha_{12}, z_1, z_2, \varphi_1, \varphi_2) =$$

$$\left(\left(z_2 \sin \alpha_{12} \sin \alpha_2 - R_c \left(\cos \alpha_2 \cos \varphi_2 \sin \varphi_2 + \sin \varphi_1 \right) \right)^2 + \right.$$

$$\left. + \left(R \sin \alpha_1 + z_2 \left(\cos \alpha_2 \sin \alpha_1 - \cos \alpha_1 \cos \alpha_{12} \sin \alpha_2 \right) + \right.$$

$$\left. + R_c \left(\cos \varphi_2 \sin \alpha_1 \sin \alpha_2 + \cos \alpha_1 \cos \alpha_{12} \cos \alpha_2 \cos \varphi_2 - \right.$$

$$\left. \cos \alpha_1 \sin \alpha_{12} \sin \varphi_2 - \cos \varphi_1 \right) \right)^2 +$$

$$\left. + \left(R \cos \alpha_1 + z_2 \left(\cos \alpha_1 \cos \alpha_2 + \cos \alpha_{12} + \cos \alpha_{12} \sin \alpha_1 \sin \alpha_2 \right) + \right.$$

$$\left. + R_c \left(\cos \alpha_1 \cos \varphi_2 \sin \alpha_2 - \cos \alpha_{12} \cos \alpha_2 \cos \varphi_2 \sin \alpha_1 + \right.$$

$$\left. \sin \alpha_1 \sin \alpha_{12} \sin \varphi_2 \right) - z_1 \right)^2 \right)^{1/2}$$

Second parameterization:

$$r(dS_{1}, dS_{2}) = r(t_{1}, t_{2}, H, \gamma, z_{1}, z_{2}, \varphi_{1}, \varphi_{2}) =$$

$$\left(\left((t_{2} + z_{2}) \sin \gamma + R_{c} (\sin \varphi_{1} - \cos \gamma \sin \varphi_{2}) \right)^{2} + \right.$$

$$\left. + \left(H + R_{c} (\cos \varphi_{2} - \cos \varphi_{1}) \right)^{2} + \right.$$

$$\left. + \left((t_{2} + z_{2}) \cos \gamma - R_{c} \sin \gamma \sin \varphi_{2} - (t_{1} + z_{1}) \right)^{2} \right)^{1/2}$$

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