DP Train, then DP Compress: Model Compression in Deep Potential Molecular Dynamics

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Machine learning based interatomic potential energy surface (PES) models are revolutionizing the field of molecular modeling. However, although much faster than electronic structure schemes, these models suffer from a lower efficiency as compared to typical empirical force fields due to more sophisticated computations involved. Herein, we report a model compression scheme for boosting the performance of the Deep Potential (DP) model, a deep learning based PES model. This scheme, we call DP Compress, is an efficient post-processing step after the training of DP models (DP Train). DP Compress combines several DP-specific compression techniques, which typically speed up DP-based molecular dynamics simulations by an order of magnitude faster, and consume an order of magnitude less memory. We demonstrate that DP Compress is sufficiently accurate by testing a variety of physical properties of Cu, H$_2$O, and Al-Cu-Mg systems. DP Compress applies to both CPU and GPU machines and is publicly available at https://github.com/deepmodeling/deepmd-kit.

I. INTRODUCTION

Deep learning is leading to a paradigm shift in molecular dynamics (MD), the de facto lens for the microscopic understanding of a broad spectrum of issues, such as drug discovery, complex chemical processes, nanotechnology, etc. Some protocols that integrate physics-based principles and advantages of deep neural networks (DNN), while retaining the accuracy of quantum mechanics (or ab initio) models, can greatly boost the accessible time and size scales by several orders of magnitude [18]. Recently, a highly optimized implementation of linear-scaling Deep Potential Molecular Dynamics (DeePMD), a deep learning-based MD scheme, has pushed the limit of molecular dynamics with ab initio accuracy to 100 million atoms, with a computational cost that typically requires one day for nano-second (ns) simulations [9, 10]. DeePMD has enabled various applications in, for example, reactive uptake of nitrogen oxides by aqueous aerosol [11], crystal nucleation of liquid silicon [12], liquid-liquid phase transition of water [13], one dimensional cooperative diffusion in three dimensional crystal [14], structural order in quasicrystal growth [15], phase diagram of water [16], and warm dense matter [17, 18], etc. However, for many important problems that require large system sizes or long time scales, the estimated computational cost is still prohibitive. For example, in order to perform a 1-ns simulation of 1 million Cu atoms using the DeePMD-kit code [10] on a machine with 150 V100 GPU cards, about half a week would be needed. Therefore, to truly make large-scale molecular simulation with ab initio accuracy a routine procedure, a major demand is to improve the efficiency of model
inference, while reducing the computational cost.

In conventional deep learning territories like speech recognition, visual object recognition, object detection, etc., it has become a common practice to conduct model compression between two stages: model training and model inference. In the training stage, the model architecture is typically large and has to be made suitable for a parameter optimization scheme to work efficiently; while after training, the computational cost for model inference may be greatly reduced without significant drop in accuracy. Popular methods to compress deep networks include parameter pruning, low-rank factorization, weight quantization, as well as some judiciously designed neural architecture search and grow-and-prune schemes [19–22]. We refer to recent review articles [24–26] for thorough discussions of related issues.

Two issues need to be addressed when the model compression techniques are used for deep learning assisted physical models. We take Deep Potential (DP) [5, 6], the interatomic potential energy model for driving DeePMD simulations, as an example. First, the accuracy requirement for DP is much more strict than conventional model compression tasks. For a system, the energy and the forces, and hence many calculated properties, predicted by the compressed DP model should show negligible differences with the original model. Second, the network structure is not as deep and large as in conventional deep learning tasks. Therefore, many existing compression techniques are not directly applicable. Not surprisingly, model compression is still a new topic, but may be an important concept, in the field of machine learning assisted scientific computing.

In this work, we introduce DP Compress, an efficient post-processing step after the training of DP models (DP Train), the resulting compressed model can be directly utilized in atomistic simulations. DP Compress combines several DP-specific compression techniques, which typically speedup the state-of-the-art DeePMD code by an order of magnitude faster, and an order of magnitude memory-efficient. We demonstrate that the error induced by the compression process is sufficiently small, and such an improvement applies to both CPU and GPU machines, so that users with different hardware environments can benefit from it. In practice, we generate compressed models for Cu, H₂O and Al-Cu-Mg alloy systems, and investigate their performances on the predictions of various physical properties, using both CPU and GPU machines. Moreover, to provide the users with a better guidance, we study in detail how the performance changes with the architectures of the neural network model.

The DP Compress scheme has been implemented in the open-source package DeePMD-kit [27], which is written in Python and C++. For efficient and flexible training, the code has been interfaced with major machine learning frameworks like TensorFlow [28]. For large-scale MD simulations, it has been interfaced with popular MD software like LAMMPS [29]. Using DP Compress, with a simple command, the users of DeePMD-kit can typically gain an order of magnitude efficiency when performing DeePMD simulations.

II. METHODOLOGY

We divide the typical DeePMD workflow into four steps. First, the preparation of the training data, which consists of a set of atomic types and atomic coordinates, as well as corresponding labels (energies, forces, and/or virials) obtained from quantum mechanical calculations. Note that an advanced scheme to generate an optimal set of training data involves a concurrent learning procedure that iteratively conduct model training, DeePMD explo-
ration, and quantum mechanics calculations (See, e.g., Refs. [30][31] for details). Second, the model training procedure with the training data, a process that optimizes the neural network parameters in a DP model. The typical training time spans from several hours to one week on a single GPU card, depending on the complexity of the data. Third, the model freezing process identifies and saves all of the required model information, including the computational graph, neural network parameters, etc., in a single file. Finally, the frozen model can be used for DeePMD simulations, during which the interatomic energies, forces, and/or virials, are calculated on-the-fly using the frozen model.

The most computationally intensive part for the DP model inference is the single-atom workflow, because the interatomic energy \( E \) is constructed as the summation of contributions from all of the atomic energies \( E^a \), i.e., \( E = \sum_a E^a \). We use \( N_i = \{j | r_{ij} < r_c \} \) to denote the set of neighboring atoms of atom \( i \) within a real-space cutoff \( r_c \) and \( r_{ij} \) denotes the distance between atoms \( i \) and \( j \). Importantly, the DP model preserves necessary symmetry properties of a PES model, i.e., translational symmetry, rotational symmetry, as well as permutational symmetry, and it is fully end-to-end. We refer to Ref. [2] for more discussions. Note that for simplicity, here we only introduce the procedure to compute \( E^a \), but similar considerations apply to the calculations of the forces and the virials, which involve the derivatives of \( E^a \) with respect to \( \alpha \).

We first construct an environment matrix \( \tilde{R}^i \) to characterize the environment of a given atom \( i \), which is illustrated in Fig. [1](a). Additionally, for each pair distance \( r_{ij} \), we introduce a weighting function \( s(r_{ij}) \), which decays smoothly to zero as \( r_{ij} \) approaches the cutoff \( r_c \). The use of \( s(r_{ij}) \) enforces a continuous evolution when atoms enter/exit the neighborhood of \( i \) by describing the atomic coordinates \( r_{ij} = (x_{ij}, y_{ij}, z_{ij}) \) with a 4-vector \( (s(r_{ij}), s(r_{ij}) x_{ij}, s(r_{ij}) y_{ij}, s(r_{ij}) z_{ij}) \), which then undergoes a normalization procedure. Furthermore, by utilizing the data sampled from the training set, we calculate the mean value and standard deviation of each element in the 4-vector. To be specific, for the first element \( s(r_{ij}) \), we subtract the mean value and divide the result by the standard deviation, and we collect all of the data and denote the whole map as \( \tilde{s}(r_{ij}) \). For the remaining three elements, since they are equivalent under arbitrary spatial rotation operations, we divide them by their overall standard deviation. After the above procedures, we denote the resulting 4-vector as \( \tilde{r}_{ij} \), which is then used to define the environment matrix \( \tilde{R}^i \).

Next, a descriptor \( D^i \) is generated based on the environment matrix \( \tilde{R}^i \). First, in the original single-atom workflow of DeePMD-kit, the rows of \( \tilde{R}^i \) are mostly given by \( \tilde{r}_{ij} \), with the neighbors \( j \) sorted first according to their types \( \alpha \), and then according to their distances to \( i \). Meanwhile, one needs to set the maximal number of neighbors of each atom type, denoted as \( sel_{\alpha} \). As a result, the number of rows of \( \tilde{R}^i \), we call the cutoff number, is fixed to be \( N_{cut} = \sum_{\alpha} sel_{\alpha} \). If the number of neighbors of type \( \alpha \) is smaller than \( sel_{\alpha} \), the remaining rows of \( \tilde{R}^i \) for that type are fed with zeros. Second, the embedding matrix \( G^i = (G^i_m) = (G^i_m(s(r_{ij}))) \), with \( N_{cut} \) rows and \( M \) columns, is generated by a DNN named embedding net. Third, multiplication of \( (G^i)^T \) by \( \tilde{R}^i \) yields the matrix \( S^i = (G^i)^T \tilde{R}^i \) with \( M \) rows and 4 columns. Let \( S^{i<} \) be the matrix formed by the first \( M' \) (\(< M \)) rows of \( S^i \). Finally, the descriptor is generated via \( D^i = S^i(S^{i<})^T \) with \( M' \) rows and \( M' \) columns. The descriptor is then passed to a fitting net, a fully connected DNN, which outputs the atomic energy contribution \( E^\alpha \).

Now, we describe the procedure to compress the single-atom workflow after training. First of all, the generation of the embedding network is the most computationally expensive part in both calculations of the forward and the backward propagation. Typically, more than 80% of the computational time is spent on this part by using either CPU or GPU machines. Essentially, by using the \( \tilde{s}(r_{ij}) \) as inputs, the trained embedding network learns a list of 1-dimensional functions. Therefore, the embedding network can be substituted with tabulated functions to largely speedup the computations. Here we adopt the piecewise fifth-order polynomials to interpolate the embedding functions. Specifically, the multi-valued embedding network can be replaced by a set of multiple single-valued functions: \( G_m, m = 1, 2, \ldots, M \). We divide the domain of the input tensor \( \tilde{s}(r_{ij}) \) into \( L \) equally spaced components, and the \( L + 1 \) interpolation points are labelled as \( x_1, x_2, \ldots, x_L, x_{L+1} \). Within the region \([x_i, x_{i+1}]\), we define a fifth-order polynomial \( f_m(x) \) according to the following formula:

\[
f_m(x) = a_m^0 x^5 + b_m x^4 + c_m x^3 + d_m x^2 + e_m x + f_m,
\]

where \( a_m^0, b_m, c_m, d_m, e_m, \) and \( f_m \) are fitting parameters.

In addition, we prepare six constraints at the two mesh points \( x_1 \) and \( x_{L+1} \) in order to compute the above six coefficients. To be specific, for each mesh point, we compute the value of the embedding function

\[
y_i = G_m(x_i),
\]

the first-order derivative

\[
y_i' = G_m'(x_i),
\]

and the second-order derivative

\[
y_i'' = G_m''(x_i).
\]

The resulting formulas for the six coefficients can be written as

\[
a_m^0 = \frac{1}{2f^2}[12\theta - 6(y_i'_{i+1} + y_i')t + (y_i'' - y_i')t^2],
\]

\[
b_m^0 = \frac{1}{2f^2}[-30\theta + (14y_i'_{i+1} + 16y_i')t + (3y_i'' - 2y_i''_{i+1})t^2],
\]

\[
c_m^0 = \frac{1}{2f^2}[-24\theta + (28y_i'_{i+1} + 30y_i')t + (3y_i''_{i+1} - 2y_i''_i)t^2],
\]

\[
d_m^0 = \frac{1}{2f^2}[-24\theta - (28y_i'_{i+1} + 30y_i')t + (3y_i''_{i+1} - 2y_i''_i)t^2],
\]

\[
e_m^0 = \frac{1}{2f^2}[12\theta + 6(y_i'_{i+1} + y_i')t + (y_i'' - y_i')t^2],
\]

\[
f_m^0 = \frac{1}{2f^2}[12\theta - 6(y_i'_{i+1} + y_i')t + (y_i'' - y_i')t^2],
\]

where \( \theta = \tilde{s}(r_{ij}) \) is the value of the embedding function at \( r_{ij} \).
\[ c'_m = \frac{1}{2t^2} [20h - (8y'_{i+1} + 12y_i)t - (3y'_i - y_{i+1})t^2], \quad (7) \]

\[ d'_m = \frac{1}{2} y'_i, \quad (8) \]

\[ e'_m = y_i, \quad (9) \]

\[ f'_m = y_i, \quad (10) \]

where \( t = x_{i+1} - x_i \) and \( h = y_{i+1} - y_i \). In practice, both \( G'_m(x_i) \) and \( G''_m(x_i) \) can be efficiently evaluated, which enables the model compression process to be finished within a few minutes on a single-node CPU machine.

The accuracy of the compressed DP model depends on the tabulation step \( \Delta t \), while the range of \( r_{ij} \) being interpolated is determined by the training data. For example, the lower bound of \( r_{ij} \), which is denoted as \( r_t \), is chosen by scanning all of the training data. In addition, the algorithm guarantees that the upper bound of \( r_{ij} \) used in the compression model is larger than the maximum value found in the training data. In this regard, the range of \( \hat{s}(r_{ij}) \) being interpolated is \([\hat{s}(r_j), \hat{s}(r_{ij})]\). As shown in Fig. 2(a), with a tabulation step of \( 10^{-2} \), the errors of energy and force can be controlled below \( 10^{-3} \) meV/atom and \( 10^{-4} \) meV/Å, respectively, much lower than the typical training errors of the DP model. Therefore, we set the default tabulation step to be \( 10^{-2} \).

In the original DP workflow, the embedding matrices from all of the atoms typically consume more than 90 percent of the total host/device memory usage \[3\], which becomes a bottleneck for simulating a larger number of atoms. Specifically, in the single-atom workflow, the embedding matrices are loaded to the registers and the matrix product \( S^i = (G')^T R^i \) is computed. The above process causes a huge data movement overhead between the registers and the host/device memory, which is memory-bound by the host/device memory throughput \[10\]. In the compressed DP workflow illustrated in Fig. 1(c), after tabulating the embedding matrix \( G' \) with fifth-order polynomials, we perform an efficient kernel fusion step to yield \( S^i \). Taking the GPU implementation as an example, for each atom \( i \), the matrix multiplication \( S^i = (G')^T R^i \) is handled by a single thread block. In detail, when one column of \((G')^T\) is evaluated and stored in registers (without storing back to global memory), the corresponding row of the environment matrix \( R^i \) is loaded into the register to perform an outer-product with the column of \((G')^T\). The outer-product has to be performed at most \( N_{cut} \) times to yield \( S^i \), which has dimensions of \( M \times 4 \).

We remark that \( G' \) neither allocated nor moved between global memory and registers in the optimized code, and both the memory footprint and computational time are significantly reduced after the kernel fusion.

In a practical simulation, the number of neighbors with type \( \alpha \) can be much smaller than \( sel_{\alpha} \), so that the environment matrix \( R^i \) may have a large number of redundant zeros. This issue is particularly serious when one trains a DP model with data in a large concentration range for a few types of atoms, so that \( sel_{\alpha} \) has to be very large for each type. In the fused kernel of matrix product \( S^i = (G')^T R^i \), the column of \((G')^T\) is evaluated and the following outer product is performed only when \( j \) is a valid neighbor of atom \( i \). This fine-grained and conditional matrix production is not possible in the original DP workflow, in which the matrix product is performed by a GEMM call. As a result, these operations reduce the floating operations per second (FLOPS) and data access at the same time.

### III. RESULTS AND DISCUSSION

We adopt three well-benchmarked systems, i.e., Cu, H\(_2\)O, and Al-Cu-Mg, to validate the DP Compress scheme. First, for the Cu system, the authors in Ref. \[31\] adopted a concurrent learning scheme \[30\] to prepare an optimal set of \( ab \) \( initio \) training data and generated a Cu model with an uniform accuracy over a wide range of thermodynamic conditions (temperatures up to \( \sim 2600 \) K and pressures up to \( \sim 5 \) GPa). Second, for the H\(_2\)O system, previous works in Refs. \[31, 32\] have shown that DeePMD can accurately capture the delicate balance between weak non-covalent intermolecular interactions, thermal effects, as well as nuclear quantum effects in water. Extensions of the DP formulation have made possible accurate predictions of the infrared \[33\] and Raman \[34\] spectra of water. More recently, part of the authors have generated a DP model to study the phase diagram of water ranging from low temperatures to about 2400 K and low pressures to 50 GPa, excluding the vapor stability region \[16\]. Last, for the Al-Cu-Mg system in the full concentration range, a DP model was generated \[35\] that yields predictions consistent with first-principles calculations for various binary and ternary systems on their fundamental energetic and mechanical properties \[35\].

We list the parameters utilized in the calculations. For Cu, H\(_2\)O, and Al-Cu-Mg, the cutoff radii \( r_c \) (number of neighbors \( N_{cut} \)) are chosen to be 8.0 Å (512), 6.0 Å (144), and 9.0 Å (1800), respectively. The size of the fitting nets are set to (240, 240, 240), while the sizes of the embedding nets are (32, 64, 128) for Cu and H\(_2\)O systems and (25, 50, 100) for Al-Cu-Mg systems. More details of these models and training data can be found in Refs. \[10, 31, 35, 36\]. We suggest that using double precision and a tabulation step of \( 0.01 \) or smaller for the DP Compress scheme. While using the above protocol for the following tests, we also study the influences of different setups on the final results, including the type of precision, the length of the tabulation step, as well as the network structure. All of the calculations are performed with the LAMMPS package \[29\] that has an interface with DeePMD-kit.
algorithms for a set of systems: Cu, H\textsubscript{2}O, and Al-Cu-Mg. (a) Root mean square errors of energy and forces as functions of the tabulation step; (b) Maximal number of atoms that can be simulated on an NVIDIA V100 GPU (32 GB memory); (c) Time-to-solution (µs/atom/step) of DP models tested on a 6-core Intel Xeon 8163 CPU; (d) Time-to-solution (µs/atom/step) of DP models tested on an NVIDIA V100 GPU. The Cu, H\textsubscript{2}O, and Al-Cu-Mg systems being tested for (a), (c), and (d) contain 6912, 12288, and 5120 atoms, respectively. For producing (c) and (d), the MD equations are numerically integrated for 500 steps (the energy and forces are evaluated for 501 times).

Fig. 3 illustrates the performances of the original and compressed models on the Cu, H\textsubscript{2}O, and Al-Cu-Mg systems. In Fig. 3(a), we adopt three tabulation steps, i.e., \(\Delta t = 0.1\), 0.01, and 0.001, to generate three compressed models for each system. We observe that the energy deviation \(\Delta E\) and force deviation \(\Delta F\) decrease as \(\Delta t\) becomes smaller, and conclude that \(\Delta t = 0.01\) is accurate enough for most DeepMDF applications. In Fig. 3(b), we compare the number of atoms that can be simulated on one single V100 GPU by using the original and compressed models. By using the compressed model, we find that the number of atoms in the Cu/H\textsubscript{2}O/Al-Cu-Mg system increases by roughly an order of magnitude. For example, the maximal number of atoms handled by one GPU increases from 12/49/5 thousands to 129/246/61 thousands for the Cu/H\textsubscript{2}O/Al-Cu-Mg system, respectively. Because the compressed DP model does not store the local embedding matrix, DeePMD is able to handle a larger number of atoms on a given machine. Meanwhile, the compressed model largely speeds up the single-atom workflow. Figs. 3(c) and (d) show that the DeePMD simulations with the compressed models are significantly faster than the original models on CPU and GPU machines, respectively. For instance, the speedups for Cu, H\textsubscript{2}O, and Al-Cu-Mg are 9.69, 3.67, and 16.22 on a single V100 GPU, respectively.

We summarize two major factors that affect the performance of DP Compress and its improvement over the original model. First, the average number of neighbors (H\textsubscript{2}O<Cu<Al-Cu-Mg) depends on the cutoff radius \(r_c\) and the density of a system; with similar network architectures, this factor roughly determines the maximal number of atoms that can be simulated on a given machine (H\textsubscript{2}O>Cu>Al-Cu-Mg in Fig. 2 (b)), as well as the ultimate time-to-solution of the compressed model (H\textsubscript{2}O<Cu<Al-Cu-Mg in Figs. 2 (c-d)). Second, the difference between the cutoff number \(N_{cut}\) and the average number of neighbors also plays an important role in determining the speed-up ratio, which explains why on both CPU and GPU, the speed-up ratio for H\textsubscript{2}O is much smaller than that for Al-Cu-Mg. On one hand, the H\textsubscript{2}O model is trained from snapshots of liquid water at ambient conditions, so the local density fluctuation is small in water and \(N_{cut}\) is close to the average number of neighbors. On the other hand, the trained DP model for Al-Cu-Mg system covers the full concentration range, so \(N_{cut}\) has to be large enough to cover extreme cases. Therefore, in practical simulations, the average number of neighbors is much smaller than \(N_{cut}\) and a substantial amount of redundant zeros exist in the environment matrix \(\mathcal{R}\); this redundant problem is well addressed by the kernel fusion procedure in the compressed model.

To validate the accuracy and applicability of the
The performances of the original and the compressed models depend on the detailed structures of the embedding net and the fitting net. To clarify this, we test a system with 4096 water molecules and the results are shown in Fig. 5. The embedding net structure is chosen to be $a-2a-4a$ with $a$ being the number of neurons, while the fitting net structure is set to $b-b-b$ with $b$ being the number of neurons. Generally speaking, a larger number of $a$ or $b$ leads to more accurate models but a lower efficiency. Notably, as illustrated in Fig. 5, we observe that the accuracy of DP models saturates when $a = 32$ and $b = 240$. In this regard, we suggest that the best network structure may be case-specific and depends on the quality and complexity of the training dataset. Furthermore, the conventional compression schemes adopted in the machine learning community, such as pruning and neural architecture search, should benefit this process, and will be considered in the future.

With the abovementioned techniques implemented in the compressed model, the computational hotspot of the compressed DP model has changed, which has profound implications. On one hand, since the embedding net is the major computational bottleneck in the original DP model, a better efficiency can be gained only if the size of the embedding net is reduced. On the other hand, in the compressed DP model, the computational costs for...
FIG. 5: Accuracy and time-to-solution (TtS) of DP models by using CPU and GPU devices with different neuron network structures. (a) Root mean square errors of energy and forces as a function of different neuron network structures. (b) Time-to-solution ($\mu$s/atom/CPU-core/step) of DP models tested on a 6-core Intel Xeon 8163 CPU. (c) Time-to-solution ($\mu$s/atom/GPU/step) of DP models tested on an NVIDIA V100 GPU. The labels on the x-axis, a-b depict the embedding net with layer sizes of a-2a-4a, and the fitting net with layer sizes of b-b-b.

IV. CONCLUSION

In summary, we propose a DP Compress scheme that can significantly boost the performance of DP models with controllable loss of accuracy. The new scheme will benefit all of the users of DeePMD-kit, as well as inspire other methodology developers in the field of machine learning assisted scientific computing. In the future, more optimizations on different operators, on the computational graph, and on multiple hardware devices, would be needed. Moreover, DP Compress can be generalized to other DP-based models, such as vectors [33] and tensors [34], without essential difficulties. With DeePMD-kit being an open-source software package, we expect that more innovative and useful schemes can be continuously integrated in the code by developers not limited to the authors, and we expect that all these later improvements can benefit the users in a timely manner.

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[1] Jörg Behler and Michele Parrinello. Generalized neural-network representation of high-dimensional potential-energy surfaces. Physical Review Letters, 98(14):146401, 2007.

[2] Stefan Chmiela, Alexandre Tkatchenko, Huziel E Sauceda, Igor Poltavsky, Kristof T Schütt, and Klaus-Robert Müller. Machine learning of accurate energy-conserving molecular force fields. Science Advances, 3(5):e1603015, 2017.

[3] Kristof Schütt, Pieter-Jan Kindermans, Huziel Enoc Sauceda Félix, Stefan Chmiela, Alexandre Tkatchenko, and Klaus-Robert Müller. SchNet: A continuous-filter convolutional neural network for modeling quantum interactions. In Advances in Neural Information Processing Systems, pages 992–1002, 2017.

[4] Justin S Smith, Olexandr Isayev, and Adrian E Roitberg. ANI-1: an extensible neural network potential with dft accuracy at force field computational cost. Chemical Science, 8(4):3192–3203, 2017.

[5] Linfeng Zhang, Jiequn Han, Han Wang, Roberto Car, and Weinan E. Deep potential molecular dynamics: A scalable model with the accuracy of quantum mechanics. Physical Review Letters, 120:143001, Apr 2018.

[6] Linfeng Zhang, Jiequn Han, Han Wang, Wissam Saidi, Roberto Car, and Weinan E. End-to-end symmetry-preserving inter-atomic potential energy model for finite and extended systems. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, Advances in Neural Information Processing Systems 31, pages 4441–4451. Curran Associates, Inc., 2018.

[7] Yaolong Zhang, Sheng Ye, Jinxiao Zhang, Ce Hu, Jun Jiang, and Bin Jiang. Efficient and accurate simulations of vibrational and electronic spectra with symmetry-preserving neural network models for tensorial properties. The Journal of Physical Chemistry B, 124(33):7284–7290, 2020.

[8] Yaolong Zhang, Ce Hu, and Bin Jiang. Accelerating atomistic simulations with piecewise machine-learned ab initio potentials at a classical force field-like cost. Physical Chemistry Chemical Physics, 23(3):1815–1821, 2021.

[9] Denghui Lu, Han Wang, Mohan Chen, Lin Lin, Roberto Car, Weinan E, Weile Jia, and Linfeng Zhang. 86 pfnps deep potential molecular dynamics simulation of 100 million atoms with ab initio accuracy. Computer Physics Communications, 259:107024, 2021.

[10] Weile Jia, Han Wang, Mohan Chen, Denghui Lu, Lin Lin, Roberto Car, Weinan E, and Linfeng Zhang. Pushing the limit of molecular dynamics with ab initio accuracy to 100 million atoms with machine learning. In Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, SC ’20. IEEE Press, 2020.

[11] Mirza Galib and David T Limmer. Reactive uptake of n2o5 by atmospheric aerosol is dominated by interfacial processes. Science, 371(6532):921–925, 2021.

[12] Luigi Bonati and Michele Parrinello. Silicon liquid structure and crystal nucleation from ab initio deep metadynamics. Physical review letters, 121(26):265701, 2018.

[13] Thomas E Gartner, Linfeng Zhang, Pablo M Piaggi, Roberto Car, Athanassios Z Panagiotopoulos, and Pablo G Debedettii. Signatures of a liquid–liquid transition in an ab initio deep neural network model for water. Proceedings of the National Academy of Sciences, 117(42):26040–26046, 2020.

[14] Yong Wang, Junjie Wang, Andreas Hermann, Cong Liu, Hao Gao, Erlo Tosatti, Hui-Tian Wang, Dingyu Xing, and Jian Sun. Electronically driven id cooperative diffusion in a simple cubic crystal. Physical Review X, 11(1):011006, 2021.

[15] Insung Han, Joseph T McKeown, Ling Tang, Cai-Zhuang Wang, Hadi Parsamehr, Zhucong Xi, Ying-Rui Lu, Matthew J Kramer, and Ashwin J Shahani. Dynamic observation of dendritic quasicrystal growth upon laser-induced solid-state transformation. Physical Review Letters, 125(19):195503, 2020.

[16] Linfeng Zhang, Han Wang, Roberto Car, and E Weinan. Phase diagram of a deep potential water model. Physical Review Letters, 120(23):236001, 2021.

[17] Yuzhi Zhang, Chang Gao, Qianrui Liu, Linfeng Zhang, Han Wang, and Mohan Chen. Warm dense matter simulation via electron temperature dependent deep potential molecular dynamics. Physics of Plasma, 27:122704, 2020.

[18] Qianrui Liu, Denghui Lu, and Mohan Chen. Structure and dynamics of warm dense aluminum: a molecular dynamics study with density functional theory and deep potential. Journal of Physics: Condensed Matter, 32:144002, 2020.

[19] Tara N Sainath, Brian Kingsbury, Vikas Sindhwani, Ebru Arisoy, and Bhuvana Ramabhadran. Low-rank matrix factorization for deep neural network training with high-dimensional output targets. In 2019 IEEE international conference on acoustics, speech and signal processing, pages 6655–6659. IEEE, 2013.

[20] Song Han, Huizi Mao, and William J Dally. Deep compression: Compressing deep neural networks with pruning, trained quantization and huffman coding. arXiv preprint arXiv:1510.00149, 2015.

[21] Hay Hubara, Matthieu Courbariaux, Daniel Soudry, Ran El-Yaniv, and Yoshua Bengio. Quantized neural networks: Training neural networks with low precision weights and activations. The Journal of Machine Learning Research, 18(1):6869–6898, 2017.

[22] Barret Zoph and Quoc V Le. Neural architecture search with reinforcement learning. arXiv preprint arXiv:1611.01578, 2016.

[23] Zhihuan Li, Eric Wallace, Sheng Shen, Kevin Lin, Kurt Keutzer, Dan Klein, and Joey Gonzalez. Train big, then compress: Rethinking model size for efficient training and inference of transformers. In International Conference on Machine Learning, pages 5968–5968. PMLR, 2020.

[24] Thomas Elsken, Jan Hendrik Metzen, Frank Hutter, et al. Neural architecture search: A survey. J. Mach. Learn. Res., 20(55):1–21, 2019.

[25] Tejalal Choudhary, Vipul Mishra, Anurag Goswami, and Jagannathan Sarangapani. A comprehensive survey on model compression and acceleration. Artificial Intelligence Review, pages 1–43, 2020.

[26] Wenhan Xia, Hongxu Yin, and Niraj K Jha. Efficient synthesis of compact deep neural networks. In 2020 57th ACM/IEEE Design Automation Conference (DAC), pages 1–6. IEEE, 2020.
[27] Han Wang, Linfeng Zhang, Jiequn Han, and Weinan E. DeePMD-kit: A deep learning package for many-body potential energy representation and molecular dynamics. Computer Physics Communications, 228:178–184, 2018.

[28] Martín Abadi, Paul Barham, Jianmin Chen, Zhifeng Chen, Andy Davis, Jeffrey Dean, Matthieu Devin, Sanjay Ghemawat, Geoffrey Irving, Michael Isard, Manjunath Kudlur, Josh Levenberg, Rajat Monga, Sherry Moore, Derek G. Murray, Benoit Steiner, Paul Tucker, Vijay Vasudevan, Pete Warden, Martin Wicke, Yuan Yu, and Xiaoqiang Zheng. Tensorflow: A system for large-scale machine learning. In 12th USENIX Symposium on Operating Systems Design and Implementation (OSDI 16), pages 265–283, Savannah, GA, November 2016. USENIX Association.

[29] S. Plimpton. Fast parallel algorithms for short-range molecular dynamics. Journal of Computational Physics, 117(1):1–19, 1995.

[30] Linfeng Zhang, De-Ye Lin, Han Wang, Roberto Car, and Weinan E. Active learning of uniformly accurate interatomic potentials for materials simulation. Physical Review Materials, 3(2):023804, 2019.

[31] Yuzhi Zhang, Haidi Wang, Weijie Chen, Jinzhe Zeng, Linfeng Zhang, Han Wang, and Weinan E. Dp-gen: A concurrent learning platform for the generation of reliable deep learning based potential energy models. Computer Physics Communications, page 107206, 2020.

[32] Hsin-Yu Ko, Linfeng Zhang, Biswajit Santra, Han Wang, Weinan E, Robert A DiStasio Jr, and Roberto Car. Isotope effects in liquid water via deep potential molecular dynamics. Molecular Physics, 117(22):3269–3281, 2019.

[33] Linfeng Zhang, Mohan Chen, Xifan Wu, Han Wang, Weinan E, and Roberto Car. Deep neural network for the dielectric response of insulators. Phys. Rev. B, 102:041121, Jul 2020.

[34] Grace M. Sommers, Marcos F. Calegari Andrade, Linfeng Zhang, Han Wang, and Roberto Car. Raman spectrum and polarizability of liquid water from deep neural networks. Phys. Chem. Chem. Phys., 22:10592–10602, 2020.

[35] Wanrun Jiang, Yuzhi Zhang, Linfeng Zhang, and Han Wang. Accurate deep potential model for the al-cu-mg alloy in the full concentration space. Chinese Physics B, 2021.

[36] Robert A. DiStasio Jr., Biswajit Santra, Zhao Feng Li, Xifan Wu, and Roberto Car. The individual and collective effects of exact exchange and dispersion interactions on the ab initio structure of liquid water. J. Chem. Phys., 141:084502, August 2014.

[37] Anubhav Jain, Shyue Ping Ong, Geoffroy Hautier, Wei Chen, William Davidson Richards, Stephen Dacek, Shreyas Cholia, Dan Gunter, David Skinner, Gerbrand Ceder, et al. The materials project: A materials genome approach to accelerating materials innovation. Apl Materials, 1(1):011002, 2013.