DistMLIP: A Distributed Inference Platform for Machine Learning Interatomic Potentials

Anonymous Author(s)

Affiliation Address email

Abstract

Large-scale atomistic simulations are essential to bridge computational materials and chemistry to realistic materials and drug discovery applications. In the past few years, rapid developments of machine learning interatomic potentials (MLIPs) have offered a solution to scale up quantum mechanical calculations. Parallelizing these interatomic potentials across multiple devices poses a challenging, but promising approach to further extending simulation scales to real-world applications. In this work, we present **DistMLIP**, an efficient distributed inference platform for MLIPs based on zero-redundancy, graph-level parallelization. In contrast to conventional space-partitioning parallelization, DistMLIP enables efficient MLIP parallelization through graph partitioning, allowing multi-device inference on flexible MLIP model architectures like multi-layer graph neural networks. DistMLIP presents an easy-to-use, flexible, plug-in interface that enables distributed inference of pre-existing MLIPs. We demonstrate DistMLIP on four widely used and state-ofthe-art MLIPs: CHGNet, MACE, TensorNet, and eSEN. We show that existing foundation potentials can perform near-million-atom calculations at the scale of a few seconds on 8 GPUs with DistMLIP.

17 1 Introduction

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Atomistic simulation has been the workhorse in computational materials and drug discovery over the recent years [Merchant et al., 2023, Jain et al., 2013, De Vivo et al., 2016]. The chemical properties and behavior of a material are essentially determined by the interactions in the given set of atomic arrangements. In the most simplified framework, one can formulate this problem as solving the function that determines the potential energy surface (PES) of a set of atoms given by $E = \phi(\vec{r_i}, C_i)$, where E is the energy, $\vec{r_i}$ and C_i are the positions and chemical identities of the atoms.

To study the material's properties, multiple fundamentally different methods have been developed to 24 obtain or construct the function ϕ . Empirical interaction rules such as the electrostatic interactions 26 and Lennard-Jones potential [Jones, 1924] qualitatively describe the bond energy between atoms, but only predict the very fundamental behavior of the materials. Classical force fields (FF) like 27 embedded atom methods [Daw and Baskes, 1984], CHARM [Vanommeslaeghe et al., 2010], and 28 Amber [Wang et al., 2004] improved the prediction of the PES by adding more descriptor terms into 29 ϕ . These classical FFs are cheap, intuitive, and explainable, but are often not accurate enough and 30 have been constructed and applied to narrow chemical domains and a few elements. Fundamentally, 31 the interactions in ϕ are determined by the electronic structure of a material and can be solved in first principles by quantum mechanics. Quantum chemical simulation methods, such as Density Functional Theory (DFT) [Perdew et al., 1996] and coupled clustering (CC) methods [Raghavachari 34 et al., 1989], enabled the ab initio calculations of atomic behavior that are much more accurate than 35 empirical methods. However, their computational complexity limits the practical use of quantum

chemical simulation methods for many realistic applications. DFT, the most widely used ab initio simulation method, scales cubically $O(N_e^3)$ with the number of electrons and is therefore limited to 38 simulating only a few hundred atoms [Beck, 2000]. Prohibitively high computational cost makes 39 DFT only useful in describing materials properties that can be learned from a small simulation cell 40 [Wang et al., 2024]. 41

Machine learning approaches such as machine learning interatomic potentials (MLIPs) open the possibility to increase simulation scale while retaining quantum chemical accuracy by building ML 43 surrogate models trained on DFT and CC data [Wang et al., 2024, Gasteiger et al., 2021, Deng 44 et al., 2023, Batzner et al., 2022, Musaelian et al., 2023, Fu et al., 2025]. Compared to feature-based 45 classical FFs, deep-learning-based MLIPs enable improved learnability to better model the PES data. Graph neural networks (GNNs), especially, have demonstrated extraordinary computational 47 efficiency and accuracy by learning both long-range and high-order atomic interactions through message passing. By design, the computation time of MLIPs scales linearly with the number of atoms 49 O(N), enabling simulations with tens of thousands of atoms at nano-second time scale.

Many materials engineering problems involve finite-sized effects like protein folding [Jumper et al., 51 2021], interfacial reactions [Du et al., 2023], particle-size effects [Shi et al., 2020], and formation of 52 nano-domains [Holstun et al., 2025]. Such systems require meso-scale simulations with upwards of 53 millions of atoms, necessitating the ability to further scale the capacity of MLIP simulations. One 54 promising solution is to expand MLIP inference from single-device to multi-device inference. Simu-55 lation packages such as LAMMPS provide ad hoc solutions for multi-GPU simulation [Thompson et al., 2022]. Multi-device simulations are realized by dividing the total simulation cell into multiple, 57 mutually exclusive, small cells for each device. Each small cell is then padded with additional atoms 58 beyond the cell boundary in order to properly calculate the energy and forces within the small cell. 59 This method, known as spatial partitioning, is based on the fundamental assumption that the force 60 field only contains short-range interactions [Plimpton, 1995]. 61

Since most MLIPs are designed to be long-ranged, expanding the number of utilized GPUs during inference time is a nontrivial task due to the necessity to distribute the large system cell across multiple devices. Currently, there exists no native multi-GPU support for GNN-based MLIPs as most MLIPs have been implemented for only single-device inference. In order to support fast, accurate, 65 and parallelizable atomistic simulations, we hereby present a distributed MLIP inference platform, 66 DistMLIP, that enables efficient multi-device inference without the need for a modified architecture or additional training. Our highlighted contributions are as follows:

- Written in standalone high performance C code, DistMLIP features an efficient, general, and versatile parallel inference platform for MLIP inference. By design, most popular MLIPs can be supported with a minimal amount of adaptation. In this work, we include benchmarking results of 4 widely used MLIPs: MACE, TensorNet, CHGNet, and eSEN.
- DistMLIP leverages graph-level partitioning that allows node and edge information to transfer between GPUs at each layer of the forward pass while still maintaining the intermediates required to perform backpropagation. This allows efficient parallelization of long-range GNN-based MLIPs, which is standard for most MLIPs today. Compared to spatial partitioning, graph partitioning has **zero redundancy**, meaning that no redundant computation is thrown away during parallel inference.
- · We implemented the distribution of both the atom graph and the augmented three-body line graph, a common graph structure used in MLIPs to encode three-body atomic interactions.
- To allow flexible usage, our implementation does not depend on a 3rd party distributed simulation library such as LAMMPS. As a result, DistMLIP supports plug-in usage of any MLIP workflow.
- All code in DistMLIP is open sourced at https://github.com/AegisIK/DistMLIP.

Related Work 85

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Machine Learning Interatomic Potentials

Machine learning interatomic potentials (MLIPs) predict the potential energy surface (PES) by inputting atomic numbers, atomic positions, and optionally the lattice, and outputting the energy and

forces of the system [Bartók et al., 2010, Zhang et al., 2018]. The most common MLIP architecture today is the graph neural network (GNN), where nodes in the atom graph represent atoms and edges in the atom graph represent the pair-wise distances between atoms that are within a pre-defined cutoff distance [Batzner et al., 2022, Simeon and De Fabritiis, 2023, Passaro and Zitnick, 2023, Gasteiger et al., 2021, Schütt et al., 2021, 2018, Smith et al., 2017]. GNN computation scales linearly with the number of atoms, as the amount of computation is associated with the neighbors within the receptive field of each atom. Some MLIPs also pass messages on top of higher-order graphs, such as threebody bond graphs, that encode angles as pairwise information between bonds [Choudhary and DeCost, 2021, Deng et al., 2023, Yang et al., 2024]. MLIPs built on top of the transformer architecture have also been introduced, where "tokens" represent individual nodes and full self attention is performed over all tokens [Liao et al., 2024, Vaswani et al., 2017]. Recently, a class of foundation potentials have been shown to generalize across diverse chemistries by pretraining on massive datasets [Chen and Ong, 2022, Deng et al., 2023, Chanussot* et al., 2021, Barroso-Luque et al., 2024, Yang et al., 2024, Merchant et al., 2023, Kaplan et al., 2025]. These pretrained foundation potentials substantially reduce the need for target-system training, and their open-sourced pretrained checkpoints serve as ready-to-use universal MLIPs.

2.2 Spatial Partitioning

LAMMPS implements multi-GPU inference via a spatial partitioning approach where the simulation space is split into mutually exclusive partitions. For each mutually exclusive partition, LAMMPS creates a second, larger partition that includes all atoms up to the interaction radius of the FF, commonly known as border or ghost nodes. This is required as the energy and force calculation of the atoms within each mutually exclusive partition requires the atomic information from all nodes within the model's interaction radius. This leads to highly redundant calculations as the computation performed on the ghost nodes is thrown away after each time step. By estimate, a 64-molecule water system calculated with a 6-layer GNN that has a 6 angstrom cutoff distance would require the computation of 20,834 ghost atoms when using spatial partitioning [Musaelian et al., 2023]. Furthermore, unlike classical FFs, most current MLIPs do not have a mature interface with LAMMPS, making spatial partitioning practically infeasible for the majority of MLIPs that have been developed.

Allegro has been developed as a strictly local, E(3)-equivariant interatomic potential that features efficient parallelization through space partitioning due to its short-range design [Musaelian et al., 2023]. Instead of performing message passing where messages are passed between nodes several times, it encodes each atom-pair's relative geometry in learned spherical harmonic components and captures many-body interactions via trainable tensor products of these features. Because of this strict locality, Allegro scales particularly well on large atomic systems – Kozinsky et al. [2023] used Allegro and LAMMPS to simulate a bulk Ag model with 100 million atoms, achieving 0.003 microseconds/atom-timestep using 128 NVIDIA-A100-80GBs.

However, strictly local models experience key limitations. The need for efficient parallelization restricts their interaction range to only a few angstroms, preventing their use on systems that require the modeling of long-range interactions [Zhou et al., 2023, Song et al., 2024, Gong et al., 2025, Cheng, 2025, Anstine and Isayev, 2023]. Furthermore, the short-range design prevents the MLIP's application from simultaneously learning diverse chemical environments. As the short-range MLIP's cutoff is often determined by the radial distribution function of one targeted material system, it is infeasible to determine a universal cutoff that works for many materials if the training dataset contains more than one chemical system. These problems raise the need for a simple, unified, and versatile API to parallelize MLIPs.

SevenNet, derived from the Nequip architecture [Batzner et al., 2022], is one of the first MLIPs that support graph-parallel inference [Park et al., 2024]. A simulation of 112,000 atoms Si₃N₄ was demonstrated by distributing the 0.84 million parameter SevenNet-0 on 8 A100-80GB GPUs. However, its graph parallel algorithm is designed to work specifically with the SevenNet implementation and is not easily transferable to other MLIP architectures. Furthermore, SevenNet's graph-parallelization relies on the combination of TorchScript and LAMMPS, making it unapplicable to simulation tasks and workflows that are not built upon LAMMPS [Larsen et al., 2017, Ganose et al., 2025, Barroso-Luque et al., 2022, Ko et al., 2025].

3 Methods

Figure 1(a) denotes the usage of DistMLIP. Public MLIP models can be easily adapted to perform 143 distributed large simulations with DistMLIP. The core infrastructure of DistMLIP is in the construction of graphs, subgraphs, and communication-related metadata. 145

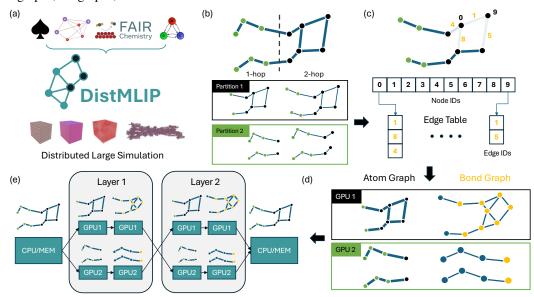


Figure 1: An overview of DistMLIP. (a) DistMLIP takes public MLIP models and performs largescale, distributed simulations. (b) Partition the atom graph using a vertical spatial partitioning scheme, and construct subgraphs containing the 1-hop neighbors and 2-hop neighbors of the original partition, which are later used to calculate the distributed bond graphs. (c) Take the 2-hop atom graph and create an edge table backbone mapping node IDs (black) to edge IDs (orange) that contain the node ID as a source node. (d) Recursively traverse the edge table to construct the atom graph and bond graph. (e) Data transfer in a simple 2-layer graph neural network with both atom graph and bond graph.

3.1 **Graph-Parallel Message Passing**

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After the material system is converted into a graph using a neighbor list construction algorithm, it can 147 be partitioned into subgraphs for each device, as illustrated in Fig. 1(b). At each graph convolution, 148 each node's features are updated according to the edge and node features of its incoming neighbors. We can partition the nodes of the graph G into p disjoint sets, constructing graphs $G_1 \dots G_n$, where p 150 is the number of partitions. Each of the graph partitions are distributed to its own GPU. To accurately calculate the features after one graph convolution, we expand G_i into G_i' , where G_i' consists of all nodes $v \in G$ such that there exists an edge $(v, u) \in E$ with $u \in G_i$. Formally, 151 152 153

$$G_i' = \{ v \in V \mid \exists u \in G_i, (v, u) \in E \},\$$

where V and E are the set of nodes and edges of the graph G, respectively. This ensures that all 154 incoming information necessary for computing the convolution is included within G'_i . Let H_i denote 155 the set of all 1-hop nodes that were added to G_i to create G'_i . Formally, 156

$$H_i = \{ v \in V \setminus G_i \mid \exists u \in G_i, (v, u) \in E \}.$$

This represents the set of nodes in V that are not in G_i but have an outgoing edge into G_i . We refer to these nodes as border nodes. Let E'_i denote the set of edges not in G'_i that point to the border nodes. 157 158 Formally, 159

$$E'_{i} = \{(u, v) \in E \mid v \in H_{i} \text{ and } (u, v) \notin G'_{i}\}.$$

 $E_i' = \{(u, v) \in E \mid v \in H_i \text{ and } (u, v) \notin G_i'\}.$ We refer to these edges as border edges, which we use extensively when distributing the bond graph. 160

After each graph convolution, we transfer the border node and border edge features to and from each 161 partition, as shown in Fig. 1(d). After this transfer process, each GPU has the most updated node and 162 edge feature to begin the next convolution. This implementation is completely model-agnostic and 163 can be applied to both conservative and direct force prediction interatomic potentials.

165 3.2 Distributing Atom Graphs

In order to distribute the atom graph, we first partition the graph spatially using vertical wall partitions. 166 Once these partitions are created, we specify algorithm 3 to identify the border nodes that each 167 partition requires as well as the border nodes within each partition that other partitions require. For 168 each partition, we create TO, FROM, and PURE arrays of node ids. We denote $TO_i[j]$ as the bucket 169 of node ids associated with G'_i required to be used in G'_i . Similarly, we denote $FROM_j[i]$ as the 170 node ids associated with G'_i required to be used in G'_i . As a result, $TO_i[j]$ and $FROM_i[i]$ should 171 be the same array. The PURE bucket specifies the nodes that are not required in the data transfer 172 process. Furthermore, each edge drawn from a border node to a pure node is assigned to the partition 173 responsible for the pure node. 174

For each partition, we concatenate each of the arrays while maintaining a marker array containing the indices of the spans of each bucket. The marker array is used to efficiently index the spans of each of the features for data transfer between GPUs. The entire atom graph creation algorithm can be found in Algorithm 1 in Appendix A. We also discuss creating, partitioning, and distributing three-body bond graphs in Appendix B.

4 Results

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In this section, we benchmark DistMLIP with the 4 MLIPs loaded with their public pretrained checkpoints: MACE-MP-0b-small-3.8M, CHGNet-2.7M, TensorNet-0.8M, and eSEN-3.2M. The details of the models and checkpoints can be found in appendix D.

For all scaling timing-related benchmarks, model inference is performed 20 times, with the average of the final 10 trials reported. This is to allow GPUs to warmup before performing calculations. We use crystalline α -quartz SiO₂ supercells for each timing benchmark, unless stated otherwise. The benchmarks are performed with a GPU cluster with 8×NVIDIA-A100-80GB-PCIe.

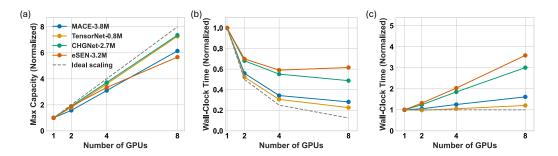


Figure 2: Performance scaling of DistMLIP inference with 4 pretrained MLIPs: MACE-3.8M, TensorNet-0.8M, CHGNet-2.7M, and eSEN-3.2M. All results are averaged over 10 inferences on a SiO₂ supercell. (a) Maximum capacity (number of simulatable atoms) vs. the number of GPUs. Values are normalized by the 1-GPU capacity. (b) Strong scaling of MLIP inference on DistMLIP, where the total number of atoms in the supercell is held constant while the number of GPUs increases. (c) Weak scaling behavior of MLIP inference on DistMLIP, where the number of atoms on each GPU device is held constant while the number of GPUs increases.

4.1 Maximum Capacity

A key performance metric is the maximum number of atoms that can be simulated by extending to multi-GPU inference. The maximum capacity scaling tests, with respect to the number of GPUs, can be found in Figure 2(a). All atom counts are normalized to be represented as multiples of the 1-GPU maximum capacity. As the number of GPUs (and thus, total GPU memory) increases, the maximum simulatable capacity increases linearly. The scaling of eSEN and MACE is further away from ideal scaling due to the one-time equivariant feature calculations that are occurring on a single GPU due to numerical stability concerns. The single GPU poses as a memory bottleneck for the system.

We also benchmark the maximum capacity and corresponding inference time against the SevenNet model while freezing model sizes, the results can be found in Appendix H.

4.2 Strong and Weak Scaling

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Strong scaling tests, where the total size of the system remains constant while the number of GPUs increases, can be found in Figure 2(b). All times are normalized to be represented as multiples of the 1 GPU time. The system sizes for MACE-3.8M, TensorNet-0.8M, CHGNet-2.7M, and eSEN-3.2M were 33.5k, 22.0k, 9.8k, and 1.4k atoms respectively. We also plot the ideal scaling under the assumption that computation performed by each GPU is purely independent and perfectly parallelizable. In particular, eSEN's high memory consumption results in small atomic cells. However, small atomic cells with partition widths that aren't sufficiently large results in overlapping border nodes during each convolution – leading to increased overhead.

Weak scaling tests, where the total size of the system increases proportionally with the number of 207 GPUs (such that each GPU performs computation on the same number of atoms), are found in Figure 208 2(c). All times are normalized to be represented as multiples of the 1 GPU time. The per GPU atom 209 count for MACE-3.8M, TensorNet-0.8M, CHGNet-2.7M, and eSEN-3.2M are 34.6k, 19.9k, 9.9k, 210 and 1.4k, respectively. In the case of eSEN-3.2M, weak scaling moves away from ideal scaling due 211 to the high constant overhead associated with initial feature calculation. For CHGNet-2.7M, the 212 computation required for the construction of the three-body graph scales with $O(N^6)$ where N is 213 the number of atoms within the three-body cutoff, leading to suboptimal weak scaling when the 214 simulation cell size increases. 215

4.3 Interaction Range

In this section, we benchmark how the parallelized simulation speed and capacity is affected by the MLIP's interaction range and number of parameters. In Fig. 3 (a), we fix each model to around 0.8M parameters and vary the number of message passing layers to increase the interaction range of the model. The 8 GPU inference is performed on the α -quartz SiO₂ of 72k atoms. The measured inference times are then divided by the inference time of the baseline 10Å version of each MLIP. eSEN ran out of memory for the 45 and 50 angstrom tests.

The results in Fig. 3 (a) show that DistMLIP only has a linear relation between parallelized inference time vs. interaction range. This is due to the additional computation cost from each increased message passing layer. Conversely, in conventional space partitioning, the volume of the simulation cell, and therefore the number of ghost atoms, grows cubically with the interaction range. This highlights the parallelization efficiency and zero calculation redundancy in graph partitioning.

228 4.4 Scaling Model Size

In Fig. 3 (b) and (c), we fix the number of message passing layers and vary the feature embedding sizes in the MLIP, therefore measuring the relation between parallelized inference speed/capacity and model parameter size. The result shows that by decreasing the model parameter size, a significant increase in simulation speed and maximum capacity can be achieved. The result suggests an estimated performance gain when distributed inference can be combined with smaller model sizes through MLIP model distillation [Amin et al., 2025].

4.5 Real World Simulations

We also show the performance of real distributed simulations on a variety of solid-state and 236 biomolecular systems, utilizing 1, 4, and 8 GPUs. The results are found in Table 1. We report 237 the microseconds/atom-timestep of each model-system pair as well as the number of simulated 238 atoms in the system. The simulated systems can be found in Figure 4. L-MACE-3.8M refers to 239 multi-GPU inference of MACE using LAMMPS spatial partitioning, while the other 4 models are 240 distributed with DistMLIP. Note that L-MACE-3.8M uses a compiled model with custom equivariant 241 CUDA kernels, while DistMLIP MACE-3.8M only runs the pure-PyTorch implementation. Custom 242 equivariant CUDA kernels have been shown to accelerate MACE inference time by up to 7.2x on 243 large models [Geiger et al., 2024]. No other model beyond MACE is reported due to the lack of LAMMPS multi-GPU inference support. We also compare DistMLIP's current partitioning strategy

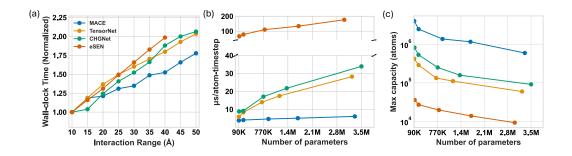


Figure 3: Effect of model configurations on graph-parallelized inference performance. (a) Inference time vs. MLIP interaction range while keeping model parameter size fixed. Values are represented as multiples of the 10Å interaction range. (b) Inference time and (c) maximum simulation capacity vs. number of parameters in the MLIP, while keeping interaction range fixed.

with METIS and RCMK graph partitioning strategies on the same real world systems while holding the rest of the DistMLIP system constant. We report those results in Table 4 in Appendix K.

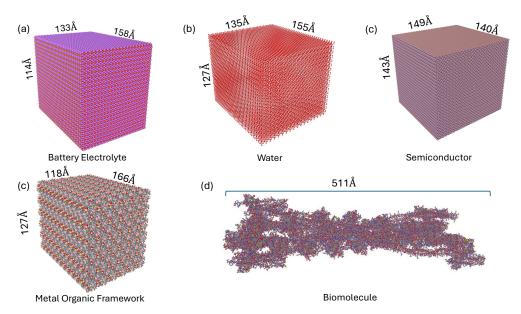


Figure 4: Sample simulation cells from real-world systems that are benchmarked in Table 1. (a) Li_3PO_4 supercell of 216.0k atoms. (b) H_2O supercell of 210.1k atoms. (c) GaN supercell of 250.0k atoms. (d) $\text{Cd}_2\text{B}_2\text{H}_{48}\text{C}_{55}\text{N}_6(\text{O}_2\text{F})_4$ metal organic framework (MOF) system of 216.0k atoms. (e) 2w49, an insect flight muscle protein of 69.3k atoms.

Our result shows that most of the current foundation potentials, even at significant model sizes of a few million parameters, are capable of simulating near-million-atom scale systems when parallelized with DistMLIP on 8 GPUs. Moreover, we noticed that the inference time, when normalized by the number of atoms, is significantly decreased when any MLIP is being parallelized. This observation suggests chemically rare events can be cheaply simulated using a larger cell for a shorter simulation time, rather than a smaller cell for a longer simulation time, which is the standard way of current atomistic simulations. As estimated from the benchmark result in table 1, nanosecond near-million-atoms simulations can be achieved at the order of 10 days with standard MLIPs and DistMLIP on a few GPUs. The max capacity of the 12Å-MACE is tripled when coupled with DistMLIP compared to LAMMPS space partitioning. For a longer-range model like CHGNet, the capacity increase and inference speed-up will be more significant as memory usage in spatial partitioning scales cubically with interaction range.

Table 1: MD step time (in μs / (atom \times step)) for the max capacity of 4 pretrained foundation potentials on DistMLIP: MACE-MP-0b-small, TensorNet-MatPES-0.8M, CHGNet-MatPES-2.7M, eSEN-3.2M. L-MACE-3.8M refers to MACE running on LAMMPS spatial partitioning. L-MACE-3.8M is a compiled model using custom equivariant CUDA kernels while MACE-3.8M uses the pure-PyTorch implementation of MACE.

Model	# GPUs	μs / (atom \times step) # of atoms (in thousands)				
		Li ₃ PO ₄	H_2O	GaN	MOF	2w49
L-MACE-3.8M	1 GPU	82.47 5.2	33.4 10.4	19.8 9.7	53.8 8.0	OOM
	4 GPUs	16.9 41.4	10.1 24.6	5.1 45.0	9.4 27.0	OOM
	8 GPUs	12.3 65.9	8.5 82.9	2.7 77.8	6.2 64.0	OOM
MACE-3.8M	1 GPU	44.8 21.9	45.9 20.7	39.5 43.9	41.0 16.0	OOM
	4 GPUs	15.3 110.6	18.2 96.0	14.6 128.0	14.7 128.0	20.1 69.3
	8 GPUs	11.0 216.0	11.6 210.1	9.6 250.0	10.9 216.0	14.0 69.3
TensorNet-0.8M	1 GPU	81.7 21.9	92.1 6.1	79.1 16.0	79.1 16.0	OOM
	4 GPUs	24.3 64	26.9 49.1	22.9 65.5	23.2 54.0	OOM
	8 GPUs	16.3 140.0	18.0 82.9	15.9 123.0	15.5 125.0	19.6 69.3
CHGNet-2.7M	1 GPU	179.7 4.1	$154.8 \mid 6.1$	100.0 5.5	174.6 2.0	OOM
	4 GPUs	94.8 21.9	80.5 20.7	$45.5 \mid 43.9$	81.1 16.0	OOM
	8 GPUs	75.4 46.7	64.5 49.1	41.9 77.8	67.1 54.0	OOM
eSEN-3.2M	1 GPU	727.3 0.9	663.2 1.3	438.9 1.0	454.3 1.0	OOM
	4 GPUs	273.4 4.1	284.0 2.6	222.3 5.5	236.3 3.0	OOM
	8 GPUs	241.2 8.0	249.1 6.1	198.9 8.2	210.0 6.0	OOM

260 5 Conclusion

Scaling the quantum-chemical simulation accuracy to realistic application scales remains a critical challenge even with recent developments of ML interatomic potentials. To address this challenge, we present DistMLIP, a distributed MLIP inference platform based on efficient graph-level partitioning. Compared to the traditional parallelization method, space-partitioning through LAMMPS, DistMLIP serves as an easy and versatile distributed inference platform that supports long-range MLIPs. DistMLIP provides infrastructures for constructing and distributing atom and bond graphs, allowing the distribution of GNN-based MLIPs that are otherwise infeasible to parallelize.

Our result shows that efficient and plug-and-play parallelization can be achieved when combining DistMLIP with existing interatomic potentials. By distributing the MLIP simulation on 8 NVIDIA-A100 GPUs, our result shows that nanosecond, near-million-atom scale simulations can be accomplished at the scale of 10 physical days with state-of-the-art MLIPs. We believe this effort to enable large-scale simulation would accelerate chemical, materials, and biological discovery.

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91 A Distributing Atom Graph

Algorithm 1 Atom Subgraph Creation **Input:** Atomic system nodes and edges **Output:** Partitioned subgraph with mappings 1. Create a partition rule based on the longest cell dimension (vertical walls) 2. Assign atoms to buckets (PURE/TO/FROM) using algorithm 3 3. Create node array and corresponding marker array for each partition: **for** each starting partition p_i (creating marker arrays) **do** initialize markers array markers[0] = 0markers[1] = len(PURE) $marker_index = 0$ **for** each destination partition p_i **do** concatenate $TO[p_i]$ to p_i node array markers[marker_index] = markers[marker_index - 1] + $len(TO[p_i])$ $marker_index = marker_index + 1$ end for **for** each source partition p_k **do** concatenate FROM[p_k] to p_i node array markers[marker_index] = markers[marker_index - 1] + $len(FROM[p_k])$ marker index = marker index + 1end for

492 B Distributing Three-body Graphs

end for

Distributing the bond graph involves selecting all 1-hop and 2-hop neighbors of the pure atom graph nodes assigned to a partition. We then create an edge table mapping from node ids to edges originating from the node id pointing to a different node. By recursively traversing the table, we are able to create the bond graph for each partition in parallel. Border nodes within the bond graph are associated with the 1-hop edge neighbors of border edges within the atom graph – hence necessitating the inclusion of 2-hop neighbors. The parallel bond graphs thus contain the 1-hop neighbors of each pure bond graph node assigned to the partition. The complete procedure is found in Algorithm 2.

Algorithm 2 depicts the method in which to distribute three-body graphs (also known as bond graphs)
as well as calculating the necessary information to perform data transfer between various partitions at
each convolution of the three-body graph.

C Assign to Partitions

Algorithm 3 is the method used to determine assign individual nodes to the PURE/TO/FROM buckets of each partition. It is used extensively in both atom graph creation (algorithm 1) and three-body graph creation (algorithm 2).

Algorithm 2 Distributed Bond Line Graph Construction

```
Input: Global edges E, partitions \{P_i\}, bond cutoff r, tolerance \tau
Output: Line graphs \{L_i\} for partitions \{P_i\}
for each partition P_i do
  Initialize TO/FROM/PURE arrays for bond graph nodes (edges within atom graph)
  Initialize edge tables T_i for each partition
  Build Edge Table T_i:
  for each edge e \in E with dist(e) \le r + \tau do
     if dst(e) in P_i then
       append e to T_i[e.src]
       if e is border edge for P_i then
          add e to FROM<sub>p_i</sub> [which_partition(e.src)]
       else if e is border edge for another partition P_j then
          add e to TO_{which\_partition(e.src)}[P_i]
       end if
     end if
  end for
  for each edge e \in E with dist(e) \le r + \tau do
     if e is pure edge assigned to P_i then
       Append e to T_i[e.src]
       add e to PURE[which partition(e.dst)]
     end if
  end for
  Localize Edges
  for each e \in T_i do
     Create mappings between global and local bond graph node indices
     Assign local node indices to each e in T_i \forall i
  end for
  Build Line Graph L_i
  for each partition P_i do
     for each v \in T_i do
       for each e \in T_i[v] do
          for each e' \in T_i[e.dst] do
             if needs_in_line(e') then
               Draw an edge in bond graph from e to e' using local node indices
             end if
          end for
       end for
     end for
  end for
end for
```

Algorithm 3 assign to partitions Subroutine

```
Input: Nodes, edges, partitions
Output: PURE, TO, FROM arrays for each partition
1. Initialize node tracking:
Create table node_to_partition[node_id] \leftarrow -1 \forall nodes
2. Populating node_to_partition
for each edge e do
  node\_to\_partition[which\_partition(e.src)] =
     which_partition(e.dst)
end for
3. Assigning nodes to partition buckets
for each node n do
  if node_to_partition[n] = -1 then
     add n to PURE array of which partition(n)
  else
     add n to \mathrm{TO}_{\mathrm{which\_partition}(n)}[\mathtt{node\_to\_partition}[n]]
     add n to FROM<sub>node_to_partition[n]</sub> [which_partition(n)]
  end if
end for
```

MLIP Versions in Benchmark 507

The table below shows the checkpoint versions of the MLIPs tested. Note that the eSEN model we 508 benchmarked is not coming from the public pretrained checkpoints of 30.2M parameters, which is too big for efficient parallelized simulation. Instead, we initialized a 3.2M eSEN in accordance with the eSEN-MPTrj-3.2M configuration found in Fu et al. [2025].

Table 2: Pretrained MLIPs Model Specifications

Model	Version	ModelSize	InteractionRange	Reference
CHGNet	matgl-MatPES-PBE-2025.2.10	2.7M	45Å	[Deng et al., 2023]
MACE	MACE-MP-0b-small	3.8M	12Å	[Batatia et al., 2023]
TensorNet	matgl-MatPES-PBE-v2025.1	0.8M	10Å	[Ko et al., 2025]
eSEN	eSEN-MPTrj-3.2M	3.2M	12Å	[Fu et al., 2025]

Single GPU Benchmarking Details

Because DistMLIP parallelizes neighbor list construction as well as underlying threebody graph 513 creation, utilizing 2 DistMLIP partitions oftentimes leads to faster total inference time and less 514 total memory consumption compared to a baseline implementation (this is especially the case 515 with CHGNet). Therefore, to maintain a fair comparison, all single-GPU results reported in any 516 benchmark utilize 2 DistMLIP partitions performing operations on the same GPU. Therefore, only 1 517 GPU is utilized, but the same fast graph creation algorithms and implementation are shared. For all benchmarking tasks, 128 threads were used for neighbor list construction and graph creation. 519

Inference Time Breakdown

Neighbor list construction could take a substantial amount of inference time when the simulated 521 system is large. In order to address this issue, we parallelized neighbor list construction in DistMLIP through multi-threading, so that graph creation time is substantially decreased compared to the single-thread neighbor list construction in Pymatgen [Ong et al., 2013]. The resulting inference time

breakdown is shown in Table 3. 525

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Table 3: Timing results (in seconds) for MACE, TensorNet, and CHGNet models across computation stages. Graph Creation consists of both DistMLIP graph creation as well as model-specific graph configuration. Feature Calculation consists of single-GPU computation overhead.

Stage	MACE	TensorNet	CHGNet
Graph Creation	0.2480	0.1262	0.3386
Feature Calculation	0.0437	0.1297	0.1018
Forward Pass	0.1701	0.1782	1.8216
Backward Pass	0.0288	0.5471	1.4074

G Scaling System Density

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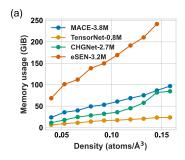
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In Fig. 5, we plot the memory consumption and inference time of scaling system density (atoms/Å³) of an SiO₂ system with 3456 atoms. DistMLIP inference with 4 A100-80GB GPUs were used. Denser atomic systems lead to a linear increase in total neighbor list size, driving up memory usage as well as inference time due to the decreased sparsity within the underlying atom graph's adjacency matrix. DistMLIP and its zero-redundancy inference algorithm scales memory consumption according to the increase in edge count.



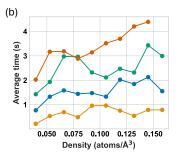


Figure 5: The effects of scaling density on (a) memory consumption, and (b) inference time. Both plots are the result of scaling atomic density (atoms/Å³) on an arbitrary system with fixed atom count using DistMLIP and 4 A100-80GB GPUs. eSEN is missing a datapoint due to out-of-memory issues.

3 H Benchmarking Against SevenNet

In this section, we benchmark the inference time and max capacity of the 4 MLIPs in DistMLIP 534 against the distributed inference of SevenNet [Park et al., 2024]. All the MLIPs are constructed to 535 have a similar number of parameters as SevenNet-0 (0.8M parameters). All tests are performed on 536 the supercells of the α -quartz SiO₂. Inference times are averaged over 10 trials after 5 warmup trials. 537 Fig. 6 shows the result for (a)SevenNet, (b)MACE, (c)TensorNet, (d)CHGNet, and (e)eSEN. The 538 number in each box in the heat map indicates the inference time of the given cell and the number 539 of GPUs, and darker color represents faster inference. Grey boxes indicate the simulation failed 540 due to the GPU out-of-memory error. We reproduced a similar maximum simulation size of 110k 541 α -quartz SiO₂ with SevenNet on 8 NVIDIA-A100-80GB, as indicated in the original manuscript. 542 Our results indicated that MACE, TensorNet, and CHGNet can generally simulate larger maximum capacity at faster speed in DistMLIP. For eSEN, all experiments failed due to the extensive memory consumption. 545

I Alignment of Single-device and Multi-device Predictions

DistMLIP's atom graph and bond graph distribution algorithms are exact in principle. However, numerical differences arise when performing computation in a distributed manner compared to on a single GPU. This is a result of non-determinism occurring during matrix multiplications and

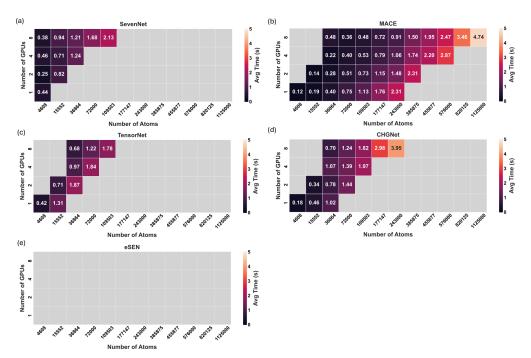


Figure 6: Inference speed and max capacity on α -quartz SiO₂. Except for (a), all other models are distributed through DistMLIP. (a) SevenNet plus LAMMPS support. (b) MACE, (c) TensorNet, (d) CHGNet, and (e) eSEN. Because SevenNet is a 0.8M parameter model, all other DistMLIP models are initialized at 0.8M parameters for comparison purposes. Grey boxes denote the inability to simulate the system either due to out-of-memory issues or system-size issues.

other operations on different GPUs. Therefore, the exact same model and weights running single GPU inference on different GPUs within the same node will also yield slightly different results. In Fig. 7, we plot the energy/atom error in meV/atom units for MACE-3.8M, TensorNet-0.8M, and CHGNet-2.7M. The result shows that the numerical error from different GPUs is far below chemical accuracy.

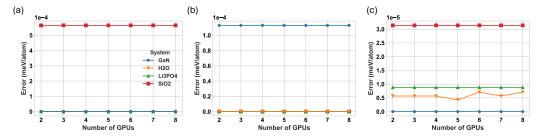


Figure 7: Energy (meV/atom) discrepancy between DistMLIP's multi-GPU inference and baseline single-GPU inference for (a) MACE-3.8M, (b) TensorNet-0.8M, and (c) CHGNet-2.7M on multiple chemical systems. Note that DistMLIP's graph partitioning and distribution algorithms are exact, and these non-perfect discrepancies are a result of non-deterministic matrix multiplication operations on different devices.

I.1 Usage

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```
# Load the MLIP as usual

chgnet = ...

from DistMLIP.implementations.matgl import CHGNet_Dist

chgnet_dist = CHGNet_Dist.from_existing(chgnet)
```

```
chgnet_dist.enable_distributed_mode([0, 1, 2, ...]) # Specify GPU ids # Run inference/simulation as usual
```

Code 1: Example code for using DistMLIP along with CHGNet. DistMLIP is designed to be a plugand-play platform for distributed inference. The current implementation only supports single-node multi-GPU inference.

564 J Parallelizing a Model in DistMLIP

DistMLIP is designed to be both high-performant as well as easily usable. Parallelizing new MLIPs using DistMLIP is a straightforward process that can be done purely in Python. A few key points of DistMLIP are outlined in J.1.

J.1 Model Parallelization Example

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```
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     Creating a DistMLIP distributed object
570
   dist = Distributed.create_distributed(...)
571
   # Distributed edge information
572
   dist.src_nodes, dist.dst_nodes # List of src and dist node pairs for
573
       each partition
574
   # Distributing node/edge features
575
   node_features_dist = dist.distribute_node_features(node_features)
576
   edge_features_dist = dist.distribute_edge_features(edge_features)
577
     Exchanging node information
578
   dist.atom_transfer(node_features_dist)
   # Aggregating node features
580
   node_features = dist.aggregate(node_features_dist)
583
```

Code 2: A subset of the available features implemented into DistMLIP. These features, implemented as a Python wrapper over efficient C and PyTorch code, allow for the straightforward distribution of any arbitrary MLIP.

K Benchmarking Partition Strategies

K.1 Graph Partitioning

Graph partitioning algorithms find applications in solving sparse linear systems of equations, circuit partitioning and layout, VLSI design, social network analysis, clustering algorithms, and image segmentation [Pothen, 1997, Stanton and Kliot, 2012, Bader et al., 2013, Tolliver and Miller, 2006, Peng et al., 2013]. One common use case in graph partitioning is to create mutually exclusive spanning sets of nodes that contain a minimum number of edges that cross from one partition to another. This use case can be tackled using sparse, symmetric matrix reordering methods such as the Reverse Cuthill-Mckee (RCMK) algorithm, which permutes a sparse matrix to minimize its bandwidth [Cuthill and McKee, 1969, Azad et al., 2017]. METIS is a graph partitioning algorithm that utilizes a graph coarsening phase, an initial partitioning sequence over the coarsened graph, and an uncoarsening and partition refinement stage [Karypis and Kumar, 1998]. However, in atomistic simulation, the underlying graphs are recalculated and repartitioned at each time step. Therefore, even small latency increases during the graph creation and partitioning stage get compounded into significant increases in overall simulation time. For MLIPs, graph parallelism has also been explored for distributed training of large, computationally expensive MLIPs Sriram et al. [2022]. We compare DistMLIP's vertical wall partitioning strategy with other common graph partitioning algorithms. In Table 4, we replace DistMLIP's current vertical wall partitioning strategy with the Reverse Cuthill-McKee (RCMK) and METIS algorithms while holding the other components of Algorithm 1 and Algorithm 3 constant. Neither RCMK nor METIS supports threebody bond graph creation. RCMK and METIS both utilize the graph's topology in order to partition the graph such that the number of crossing edges between partitions is minimized. DistMLIP's current partitioning strategy, on the other hand, doesn't perform graph traversals but rather uses atomic positions as a heuristic in order to partition the graph. In Table 4, we also include the LAMMPS spatial partitioning results for comparison. As a result, we perform all benchmarks with the MACE-3.8M model.

Table 4: MD step time (in μs / (atom \times step)) for various graph and spatial partitioning strategies. RCMK refers to the Reverse Cuthill-McKee algorithm used for graph partitioning. Both RCMK and METIS still utilize the DistMLIP platform, only the partitioning strategy is replaced. The model used was MACE-3.8M, and LAMMPS spatial partitioning values are included for comparison.

Method	# GPUs	$\mu s / (atom \times step) \mid # of atoms (in thousands)$				
		Li ₃ PO ₄	H_2O	GaN	MOF	2w49
METIS	4 GPUs 8 GPUs	81.19 108.0 62.18 216.0	101.67 96.0 56.76 216.0	$68.98 77.0 \\ 77.15 207.0$	$\begin{array}{c c} 83.60 & & 125.0 \\ 69.63 & & 216.0 \end{array}$	
RCMK	4 GPUs 8 GPUs	77.49 110.0 57.22 216.0	98.02 96.0 $51.67 216.0$	$66.92 77.0 \\ 74.01 207.0$	$\begin{array}{c c} 82.24 125.0 \\ 65.74 216.0 \end{array}$	
LAMMPS	4 GPUs 8 GPUs	$16.90 41.4 \\ 12.30 65.9$	$10.10 24.6 \\ 8.50 82.9$	5.10 45.0 $2.70 77.8$	$9.40 \mid 27.0$ $6.20 \mid 64.0$	OOM OOM
Vert. wall	4 GPUs 8 GPUs	15.30 110.6 11.00 216.0	18.20 96.0 11.60 210.1	$14.60 128.0 \\ 9.60 250.0$	$\begin{array}{c c} 14.70 & 128.0 \\ 10.90 & 216.0 \end{array}$	