Article

Integrating Local Runtime Geometry and Global Equivariant Channels for 3D Molecular Representation Learning

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Abstract: Equivariant graph neural networks have greatly advanced the development of machine learning molecular force fields, achieving molecular dynamics simulations with near quantum chemical accuracy. As an efficient vector-scalar interactive equivariant model, ViSNet relies on runtime geometric calculation (RGC) to implicitly extract local geometric information such as bond angles, dihedral angles, and improper angles with linear complexity, achieving excellent performance on small and medium-sized molecular datasets. However, native ViSNet only relies on local neighborhood message passing within a cutoff radius, meaning long-range interactions can only propagate indirectly by stacking multiple network layers. In large molecules and flexible protein systems, this easily leads to vanishing gradients and over-smoothing of representations, limiting its modeling capacity for long-range conformational spaces. This paper proposes G-ViSNet, which introduces an equivariant global scalar-vector distributing-aggregating mechanism into every ViS-MP block of ViSNet to construct a low-cost global information interaction pathway. Experiments conducted on the MD17 small molecule benchmark and MD22 large molecule benchmark datasets show that G-ViSNet exhibits no performance degradation on small molecules and significantly improves the prediction accuracy of energy and forces for large molecules. G-ViSNet balances local geometric feature extraction and long-range information modeling, providing an efficient solution for machine learning molecular dynamics simulations of flexible biological macromolecules.

Keywords: Machine learning force field; Equivariant graph neural network; ViSNet; Global message passing; Molecular dynamics

1. Introduction

Molecular dynamics (MD) simulations are core tools for understanding chemical reactions, protein conformational changes, and material transport properties [1,2]. Density Functional Theory (DFT) can provide high-precision potential energy and atomic forces, but its high computational cost restricts its application to small systems and short-time simulations. Classical empirical force fields are computationally fast, but they rely heavily on manually fitted analytical functions, making it difficult to describe complex electronic effects. Machine Learning Interatomic Potentials (ML-IPs) offer a compromise: training neural networks on first-principles datasets balances quantum accuracy with simulation efficiency, and has seen rapid development in recent years.

Equivariant Graph Neural Networks are one of the most important branches of machine learning force fields. The internal features of these models satisfy $E(3)$ Euclidean transformation equivariance; when the input molecule undergoes translation or rotation, vector outputs transform synchronously according to physical rules, allowing the model to learn 3D molecular geometric information without additional data augmentation. Existing equivariant force fields can be divided into two categories: one category is based on higher-order spherical harmonic tensors and Clebsch-Gordan tensor products, with representative works including NequIP and MACE, which possess strong

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expressive power, but the Clebsch-Gordan products incur massive computational overhead, making direct application to large molecules and protein systems difficult; the other category uses only first-order scalar-vector dual representations, such as PaiNN, ViSNet, and E²GNN, avoiding expensive higher-order tensor operations and achieving higher inference efficiency [3-7].

ViSNet is a recently proposed efficient equivariant molecular force field, with its core innovations being Runtime Geometric Calculation (RGC) and ViS-MP vector-scalar interactive message passing. The RGC module relies on vector inner products to implicitly extract geometric information of bond angles, dihedral angles, and improper angles with $O(N)$ linear complexity, breaking free from the $O(N^2)$ and $O(N^3)$ complexities introduced by traditional models through explicit traversal of triplets and quadruplets. ViS-MP achieves bidirectional interaction between node scalar features and equivariant vector features, yielding excellent results on multiple benchmarks like MD17, QM9, and Molecule3D, as well as performing molecular dynamics simulations for the Chignolin mini-protein. However, ViSNet's message passing is strictly restricted to local neighborhoods within a cutoff radius, requiring long-range interactions to propagate layer-by-layer by stacking multiple ViSNet blocks. As the number of network layers increases, vanishing gradients and representation over-smoothing easily occur, creating a modeling bottleneck for systems with substantial non-local interactions across space, such as large molecules, peptides, and proteins in MD22.

To address the limitation of long-range information propagation caused by local message passing, researchers have proposed various solutions. MACE constructs higher-order many-body messages to obtain higher-order many-body features with fewer layers, reducing reliance on network depth; however, it still depends on tensor product operations, incurring high computational costs. E²GNN proposes a global scalar-vector distributing-aggregating framework: it maintains global entities (a global scalar and a global equivariant vector), broadcasts global features to all atomic nodes at each layer, and, after completing local message updates, aggregates all node features back into the global entities. This establishes a global communication pathway across all atoms, significantly improving performance on catalytic and condensed-phase systems. However, native E²GNN adopts a direct force-prediction paradigm where output forces do not satisfy energy conservation, requiring reliance on thermostats during long-time molecular dynamics simulations, making its physical completeness weaker than conservative potential models (where forces are derived from potential energy derivatives).

Based on the current state of research, this paper proposes G-ViSNet, which integrates the global scalar-vector distributing-aggregating mechanism of E²GNN into ViSNet. We fully retain ViSNet's RGC runtime geometric calculation, Scalar2Vec/Vec2Scalar modules, and ViS-MP vector-scalar interaction logic. Simultaneously, rather than directly predicting forces, we maintain an energy-conserving potential energy framework where forces are derived by taking the derivative of potential energy with respect to atomic coordinates, avoiding E²GNN's non-conservative force defect. Inside each ViSNet block, a new global workflow is added: Global Message Distributing → Native ViSNet Block Calculation → Global Message Aggregating. This enables direct information exchange between global entities and all atomic nodes at every layer, alleviating vanishing gradients and representation over-smoothing caused by deep stacking, thereby enhancing the model's capacity to capture long-range interactions. The main contributions of this paper are summarized as follows:

1. We propose G-ViSNet, which integrates E²GNN's equivariant global scalar-vector distributing-aggregating module into ViSNet, retaining all of ViSNet's local geometric modeling capabilities. It maintains a conservative potential energy framework, addressing native ViSNet's shortcomings in long-range information propagation while avoiding E²GNN's physical defect of direct force prediction.

2. We strictly ensure the $E(3)$ equivariance of the global module and provide a mathematical proof of the rotation and translation equivariance of the global module in

the appendix. We design comprehensive ablation experiments to explore the individual contributions of global scalars and global vectors to performance while evaluating changes in computational overhead brought by the module.

3. We validate the proposed method on the MD17 and MD22 large-molecule datasets. Experimental results demonstrate that G-ViSNet significantly improves the prediction accuracy of energy and forces for large molecules without degrading performance on small molecules.

2. Related Works

2.1. Equivariant Machine Learning Molecular Force Fields

Machine learning interatomic potentials aim to learn the mapping from atomic coordinates to potential energy and atomic forces from DFT first-principles data, representing a rapidly developing direction in the field of molecular simulation. Graph neural networks based on $E(3)$ equivariance can naturally adapt to 3D molecular geometry without manual descriptors, becoming the mainstream technological route. Mainstream equivariant models are divided into two major branches:

(1)Higher-order spherical harmonic and tensor product models: The first category employs higher-order spherical harmonics and Clebsch--Gordan (CG) tensor products, supporting higher-order tensor representations ($l \geq 2$), with representative works including NequIP, MACE, and Allegro [8]. NequIP relies on higher-order equivariant convolutions and possesses high data efficiency, achieving excellent performance in both molecular and solid systems, but CG tensor products bring massive computational overhead, making it difficult to handle large-scale protein molecules. MACE constructs higher-order many-body messages to decouple the many-body order from the number of network layers, requiring only a few network layers to achieve high many-body expressive power and reducing reliance on depth; however, it still depends on tensor product operations, leaving inference costs relatively high.

(2)First-order scalar-vector dual representation models: The second category consists of first-order scalar-vector dual representation models, which only use scalar ($l = 0$) and vector ($l = 1$) features, discarding expensive higher-order CG products and relying on vector inner products to extract geometric information, with representative works being PaiNN, ViSNet, and E²GNN. PaiNN establishes bidirectional scalar-vector message passing, achieving excellent results on molecular benchmarks; ViSNet further proposes RGC runtime geometric calculation, utilizing vector rejection and inner products to implicitly encode bond angles, dihedral angles, and improper angles with linear complexity, which drastically reduces computational costs compared to explicit triplet/quadruplet traversal and exhibits outstanding performance in molecular dynamics tasks. E²GNN also adopts scalar-vector dual representations and innovatively introduces a global message distributing-aggregating mechanism, building a global-local mixed message passing framework; however, E²GNN chooses to directly output atomic forces, failing to guarantee energy conservation, which limits its application in long-time molecular dynamics simulations.

2.2. Long-Range Interaction Modeling Strategies

Local message passing within a cutoff radius is the foundational paradigm for the vast majority of graph molecular force fields, but long-range interactions beyond the cutoff radius can only rely on multi-layer message passing for gradual diffusion, leading to vanishing gradients and over-smoothing of representations. Existing works mitigate this issue from multiple angles:

(1) Elevating the many-body order of a single layer: As in MACE, constructing higher-order many-body messages within a single layer reduces the required number of network layers, indirectly lowering the number of layers needed for long-range information propagation, though single-layer computational overhead rises.

(2) Explicitly introducing physical long-range correction terms: Some models superimpose Coulomb and van der Waals analytical long-range terms at the network

output to explicitly model electrostatic long-range interactions, but this requires additional physical priors, limiting universality.

(3) Global virtual node / global entity message passing: E²GNN employs global scalar + global vector entities to perform global-local information interaction at each layer, establishing global communication at a lower cost without increasing the cutoff radius. Distinguishing itself from simple virtual nodes, E²GNN simultaneously maintains equivariant vector features to guarantee overall $E(3)$ symmetry, but this mechanism has not yet been applied to vector-scalar interactive models with conservative potential energies.

2.3. ViSNet Model and Existing Limitations

Relying on the RGC module, ViSNet can efficiently extract geometric features of local angles, dihedral angles, and improper angles; ViS-MP achieves bidirectional scalar and vector feature updates, while its energy-conserving potential design ensures molecular dynamics stability. However, all of ViSNet's message passing is restricted to the local neighborhood within the cutoff radius, lacking a direct information pathway across global atoms. When processing large molecular systems such as MD22 and Chignolin, long-range conformational information must propagate gradually through multiple network layers, easily leading to information attenuation, leaving room for improvement in model performance.

Positioning of this work: We draw on E²GNN's global scalar-vector distributing-aggregating architecture and adaptively integrate it into ViSNet. We fully retain ViSNet's efficient RGC geometric extraction and ViS-MP vector-scalar interaction while preserving the physical paradigm of conservative potential energy (where force is the negative gradient of potential energy), thereby making up for native ViSNet's shortfalls in long-range modeling and obtaining G-ViSNet, which balances local geometric representation, long-range interactions, and simulation stability. Distinguishing itself from higher-order tensor models like MACE, this work does not introduce CG products, maintaining inference efficiency; distinguishing itself from native E²GNN, it preserves energy conservation, making it suitable for long-time molecular dynamics simulations.

3. Methodology

3.1. Overall Architecture

This paper proposes an equivariant molecular graph neural network integrating a global message interaction mechanism, denoted as Global-ViSNet (G-ViSNet). Building upon ViSNet as the foundational network, this model introduces the Global Message Distributing (GMD) and Global Message Aggregating (GMA) mechanisms from E²GNN to establish a global information communication channel across the entire molecular graph while preserving ViSNet's original local geometric modeling capabilities.

ViSNet represents molecules as 3D geometric graphs and updates them iteratively via node scalar representations, vector representations, and edge geometric information. Its RGC module can implicitly extract higher-order geometric information such as bond angles, dihedral angles, and improper angles at a low computational cost, while ViS-MP achieves further fusion of geometric information through interactions between scalars and vectors. In the original ViSNet, node information primarily propagates through local neighborhoods, so the long-distance information a node can acquire relies on gradual diffusion via multi-layer message passing. E²GNN pointed out that simply increasing the number of GNN layers, although expanding the receptive field, may lead to problems such as vanishing gradients, representation over-smoothing, and optimization instability; therefore, global scalars and global vectors are introduced as graph-level communication media (As shown in Figure 1).

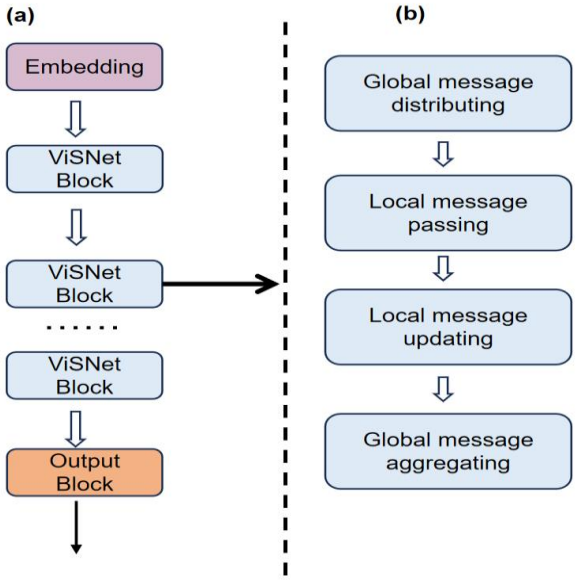

Figure 1. Overall Framework of G-ViSNet. (A) Workflow of G-ViSNet. (B) Flowchart of a G-ViSNet Block. A G-ViSNet Block Consists of Four Parts: Global Message Distributing, Local Message Passing, Local Message Updating, and Global Message Aggregating, Where the Local Message Passing and Local Message Updating Are Consistent with Those in the Baseline ViSNet Block.

3.2. Geometric Feature Construction

Given a molecular graph $G = (V, E)$, the node set V contains N atoms, where each atom i has an atomic number Z_i and 3D coordinates $\mathrm{r}_i \in \mathbb{R}^3$.

3.2.1. Node and Edge Feature Initialization

First, the atomic number is mapped to an initial scalar feature $\mathrm{x}_i^{(0)} \in \mathbb{R}^C$ via a learnable embedding layer. Subsequently, a local adjacency graph is constructed based on the cutoff radius (r_c), and the interatomic distance $r_{ij} = \|\mathrm{r}_j - \mathrm{r}_i\|$ and unit direction vector $\hat{\mathrm{d}}_{ij} = \frac{\mathrm{r}_j - \mathrm{r}_i}{r_{ij}}$ are calculated. To ensure a smooth transition of functions, distances are encoded into Radial Basis Function (RBF) features combined with a cosine cutoff function:

$$\phi(r_{ij}) = \mathrm{RBF}(r_{ij}) \cdot f_{\mathrm{cut}}(r_{ij}) \quad (1)$$

The edge feature f_{ij} is further non-linearly transformed through an Edge Embedding network.

3.2.2. Global State Initialization

The network maintains not only local features but also an independent graph-level global scalar state $\mathrm{s}_g \in \mathbb{R}^C$ and global vector state $\mathrm{v}_g \in \mathbb{R}^{V \times C}$. Here, $\mathrm{s}_g^{(0)}$ is initialized as learnable parameters, while to strictly satisfy $O(3)$ equivariance requirements, the initial global vector $\mathrm{v}_g^{(0)}$ must be initialized as an all-zero tensor.

3.3. Bidirectional Global-Local Interaction

In each layer l of the network, feature updates follow the alternating paradigm of "Global Distributing → Local Calculation → Global Aggregating".

3.3.1. Equivariant Global Vector Interaction

Because vector features carry directional information, any non-linear activation functions or biases would destroy their rotational equivariance. Therefore, in the interaction between the global vector v_g and local vectors v_i, we strictly employ linear projections without bias.

Global-to-Local:

$$\mathrm{v}_i' = \mathrm{v}_i + \mathrm{W}_{\mathrm{node}}(\mathrm{v}_i + \mathrm{v}_g) \quad (2)$$

Local-to-Global: After local feature updates are completed, the global node pools all local vectors to update itself:

$$v_g' = v_g + W_{vn}\left(\frac{1}{N}\sum_{i=1}^{N} v_i' + v_g\right) \quad (3)$$

where W_{node} and W_{vn} are learnable weight matrices. Because this involves only linear superpositions and scalar multiplications of vectors, if the input system undergoes a rotation $R \in SO(3)$, the global and local features synchronously undergo the identical rotational transformation, perfectly maintaining the equivariance constraint.

3.3.2. Global Scalar Interaction

For rotationally invariant scalar features x_i and s_g, we employ a two-layer Multilayer Perceptron (MLP) with SiLU activation functions for deep non-linear feature fusion:

$$x_i' = x_i + \mathrm{MLP}_{node}(x_i \parallel s_g) \quad (4)$$

$$s_g' = s_g + \mathrm{MLP}_{vn}\left(\frac{1}{N}\sum_{i=1}^{N} x_i' \parallel s_g\right) \quad (5)$$

where $\parallel$ denotes feature concatenation along the channel dimension. This residual connection mechanism effectively alleviates the vanishing gradient problem in deep networks.

3.4. Local Equivariant Attention Mechanism

After completing the "global-to-local" information distribution, the model propagates features within the local geometric graph through an improved ViS_MP (Message Passing) module. This component is inspired by Transformers but generalized to 3D geometric space.

3.4.1. Geometry-Aware Attention Weight Calculation

For a center node i and its neighbor j, scalar features are mapped to Query (q_i), Key (k_i), and Value (v_i) features via linear layers. Simultaneously, edge geometric features f_{ij} are mapped into distance-dependent modulating factors dk and dv . The attention weight α_{ij} between two nodes is calculated as:

$$\alpha_{ij} = \mathrm{Act}\left(\sum_c q_{i,c} \cdot k_{j,c} \cdot dk_{ij,c}\right) \cdot f_{cut}(r_{ij}) \quad (6)$$

where the introduction of the cutoff function $f_{cut}(r_{ij})$ ensures the smoothness of molecular boundary information, preventing abrupt changes in energy and forces when atoms enter or exit the cutoff radius.

3.4.2. Vector Rejection and Higher-Order Geometry

To extract many-body interactions (such as bond angles), we make extensive use of vector rejection techniques in the ViS_MP_Vertex_Edge and Node variants. Given a node vector v and an edge unit vector $\hat{d}_{ij}$, its component orthogonal to $\hat{d}_{ij}$ is computed as:

$$v_\perp = v - (v \cdot \hat{d}_{ij})\hat{d}_{ij} \quad (7)$$

By calculating dot products between orthogonal projections of vectors in different directions (e.g., $w_{dot} = w_1 \cdot w_2$), the model implicitly encodes angular information between adjacent edges. This drastically reduces computational complexity without explicitly constructing triplet graphs while retaining higher-order geometric expressiveness.

3.4.3. Coupled Update of Scalar and Vector

In the message aggregation phase, the local feature increments Δx_i and Δv_i are calculated through the mutual coupling of scalars and vectors:

- Vector Update: It not only aggregates neighboring vectors v_j but also introduces directional vector components $s_2 \cdot \hat{d}_{ij}$ predicted by the scalar network.
- Scalar Update: Rotationally invariant scalar quantities are generated via vector dot products ($v_1 \cdot v_2$) and injected into the update channels of scalar features. This scalar-vector coupling mechanism ensures continuous information exchange between structural deformation and chemical properties.

3.5. Normalization and Readout

To stabilize deep network training, scalar features use standard LayerNorm at the end of each layer. Meanwhile, because vector features must preserve directional

invariance, a specialized vector layer normalization (VecLayerNorm) is applied to normalize only their magnitudes (norms):

$$v_{norm} = \frac{v}{\|v\|+\epsilon} \cdot \gamma \quad (8)$$

After L layers of iterative propagation, the network extracts the final representations $x^{(L)}$ and $v^{(L)}$, which integrate long-range global context with precise local geometric structure. These are subsequently mapped by an output head to predicted physicochemical properties such as the target molecule's energy, dipole moment, and polarizability.

4. Experimental Analysis

4.1. Evaluation Metrics

To comprehensively evaluate the performance of the improved ViSNet incorporating the global message distributing and aggregating mechanisms (hereinafter referred to as Global-ViSNet) in predicting molecular conformational properties, we conducted energy and force prediction experiments on two widely used molecular dynamics benchmark datasets-MD17 and MD22 [9,10]. The experiments aim to verify: (1) whether the introduction of global nodes interferes with the originally efficient local feature representation in small molecular systems; and (2) whether the bidirectional global-local interaction mechanism can effectively capture long-range interactions and improve model accuracy in large molecular systems.

4.2. MD17

On the MD17 dataset, we compared Global-ViSNet with the original ViSNet model. As shown in Table 1, the experimental results indicate that the energy and force prediction mean absolute errors (MAE) of Global-ViSNet across all small molecules are virtually on par with those of the original ViSNet, reaching current state-of-the-art (SOTA) performance.

Table 1. Mean Absolute Errors (MAE) of Energies (Kcal Mol) and Forces (Kcal Mol Å) for 8 Small Organic Molecules in MD17

Model	Aspirin		Ethanol		Malondialdehyde		Naphthalene		Salicylic acid		Toluene		Uracil	
	Energy	Forces	Energy	Forces	Energy	Forces	Energy	Forces	Energy	Forces	Energy	Forces	Energy	Forces
ViSNet	0.116	0.155	0.051	0.060	0.075	0.100	0.085	0.039	0.092	0.084	0.074	0.039	0.095	0.062
G-ViSNet	0.114	0.150	0.049	0.060	0.077	0.103	0.080	0.039	0.091	0.088	0.077	0.040	0.099	0.063

4.3. MD22

As shown in Table 2, in sharp contrast to the results on MD17, G-ViSNet demonstrates a significant performance advantage on the more challenging MD22 dataset. For molecules with larger system sizes, higher flexibility, and prominent long-range van der Waals and electrostatic interactions, both the energy and force MAEs of G-ViSNet are significantly lower than those of the original ViSNet.

Table 2. | Mean Absolute Errors (MAE) of Energy (Kcal/mol) and Force (kcal/mol/Å) for 7 Large-Scale Molecules on MD22

Model	Ac-Ala3-NHMe		AT-AT		AT-AT-CG-CG		DHA		Buckyball catcher		Stachyose		Double-walled nanotube	
	Energy	Forces	Energy	Forces	Energy	Forces	Energy	Forces	Energy	Forces	Energy	Forces	Energy	Forces

ViSNet	0.064	0.083	0.071	0.081	0.196	0.148	0.074	0.060	0.508	0.184	0.092	0.088	0.800	0.362
G-ViSNet	0.055	0.070	0.062	0.069	0.181	0.139	0.067	0.053	0.421	0.169	0.080	0.077	0.723	0.349

5. Conclusion

This paper proposes G-ViSNet, which incorporates the equivariant global scalar-vector message distributing-aggregating module of E²GNN into the ViSNet model. G-ViSNet completely inherits ViSNet's Runtime Geometric Calculation (RGC) module and ViS-MP vector-scalar interactive message passing mechanism. Simultaneously, it maintains an energy-conserving potential energy framework where atomic forces are obtained by taking the derivative of the potential energy with respect to coordinates, avoiding the non-conservative force defect caused by E²GNN's direct force prediction. By adding a global message distributing-aggregating workflow within each ViSNet block, information exchange between global entities and all atomic nodes can be realized at every layer, alleviating vanishing gradients and representation over-smoothing caused by multi-layer local message passing, thereby enhancing the model's capacity to model long-range interactions in large molecules and flexible systems.

This work still has certain limitations. Consistent with the original analysis of E²GNN, global entities may introduce spurious cross-molecular signals between two independent, non-interacting sets of molecules within a simulation box; future work could introduce a gating weight mechanism to adaptively control the contribution of global information. Additionally, restricted by the foundational ViSNet architecture, G-ViSNet likewise does not satisfy geometric Weisfeiler-Leman completeness; future work could incorporate lightweight higher-order tensor operations to further enhance its expressive power.

Future research directions include: extending G-ViSNet to periodic solids and catalytic surface systems; incorporating active learning strategies to reduce the data requirements for large-molecule training sets; and further optimizing global gating mechanisms to suppress spurious interactions in isolated systems, paving the way for long-time molecular dynamics simulations on larger-scale protein systems.

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Conflicts of Interest: The authors declare no conflict of interest.

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