Geometric Graph Neural Diffusion for Stable Molecular Dynamics Simulations

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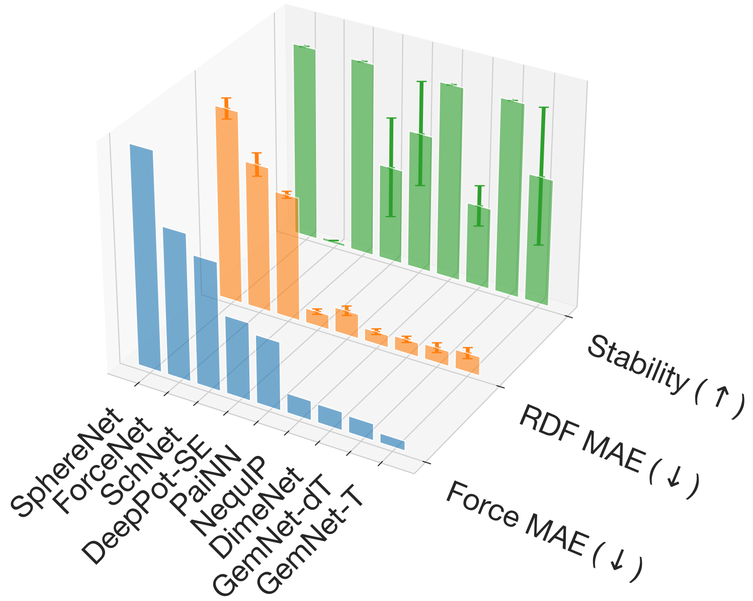
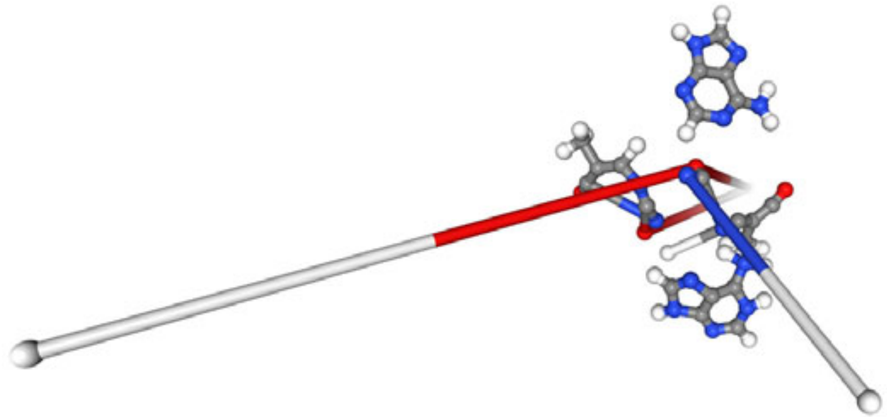
Motivation: stable molecular dynamics (MD)

- Existing Geo-GNNs for MD simulations are designed to minimize the energy MAE and force MAE.

- As shown below, lower error could still incur unstable simulations due to extreme forces from local pathological [1].

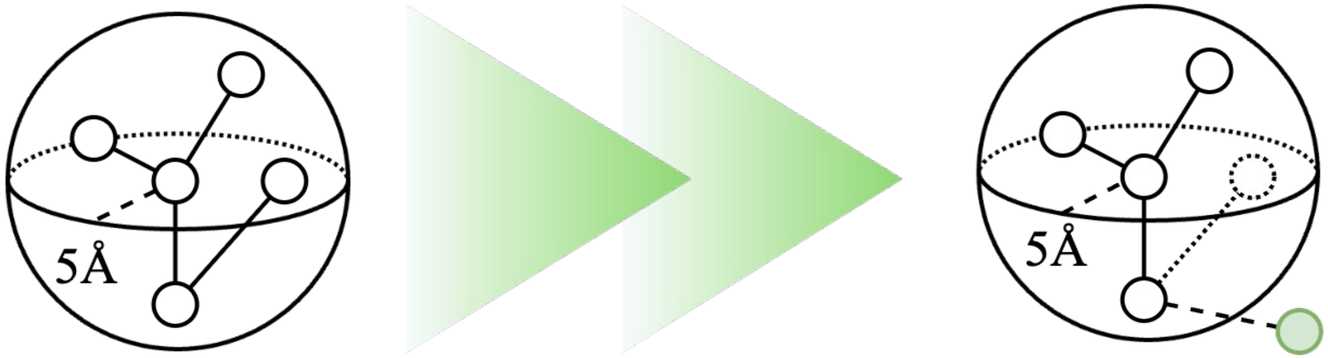




Unstability: quantified by bonding connectivity

[1] Fu, Xiang, et al, “Forces are not Enough: Benchmark and Critical Evaluation for Machine Learning Force Fields with Molecular Simulations”, TMLR, 2023

Why instability occurs: existing methods only model local neighborhoods (cutoff-induced edges), missing global structure, incapable of generalizing to unseen conformations

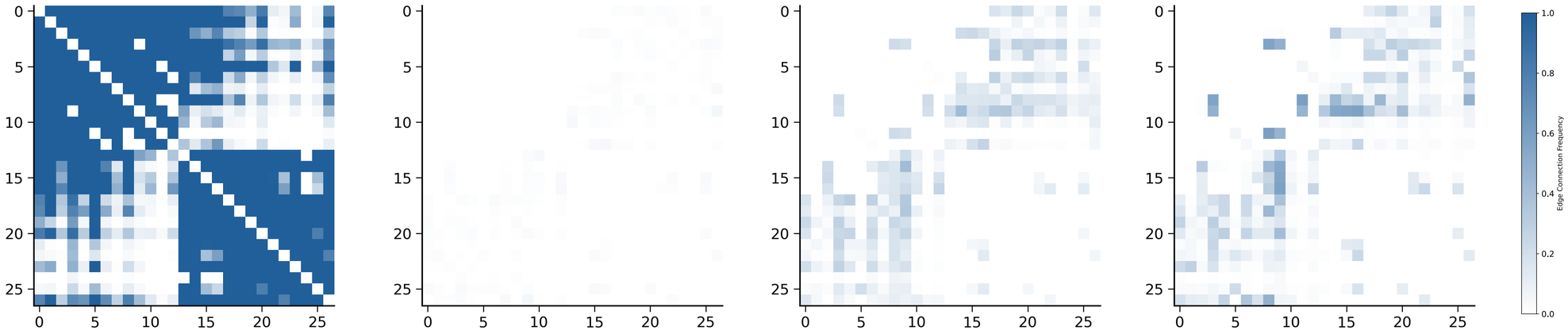


Geometric Topological Shift

Preliminary results of existing methods with OOD conformations

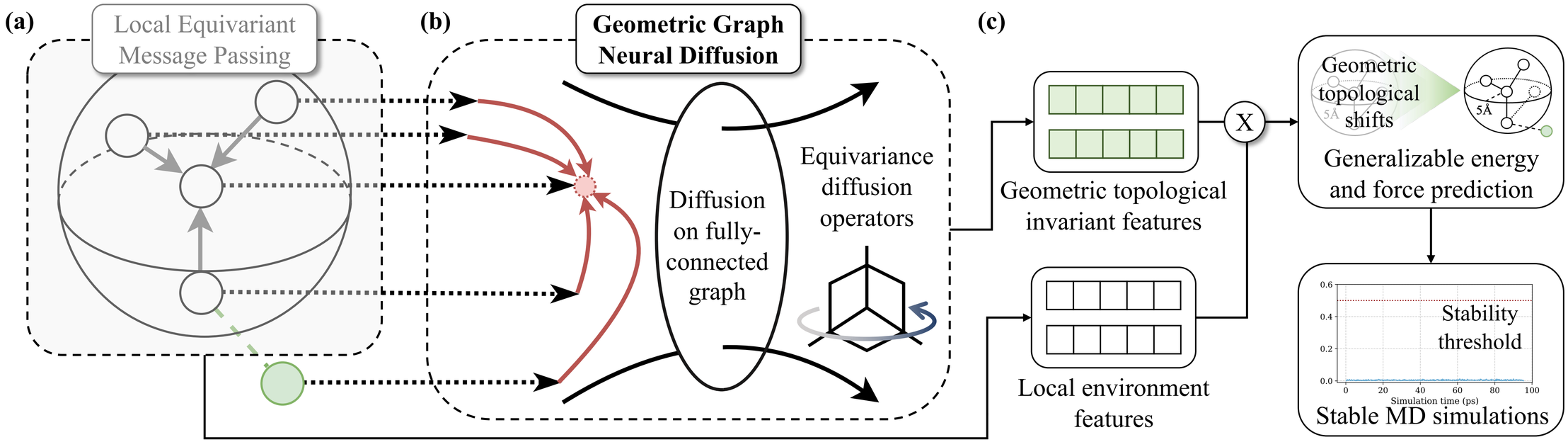
Significant stability drop

Training Set in 300 K	300 K			600 K			1200 K		
Metrics	Energy ↓	Force ↓	Stability ↑	Energy ↓	Force ↓	Stability ↑	Energy ↓	Force ↓	Stability ↑
VisNet	0.0022	0.0065	100	1.4053	0.9971	25.358	3.4642	1.4043	0.004
SEGNO	0.5925	0.3592	99.812	0.9082	0.8925	59.892	2.8359	1.2375	0.009



Our GGND: Geometric Graph Neural Diffusion

- A hybrid solution to address the geometric topology shifts
  - Equivariant local message passing to model short-range interactions
  - Equivariant diffusion on fully-connected graph to capture global information

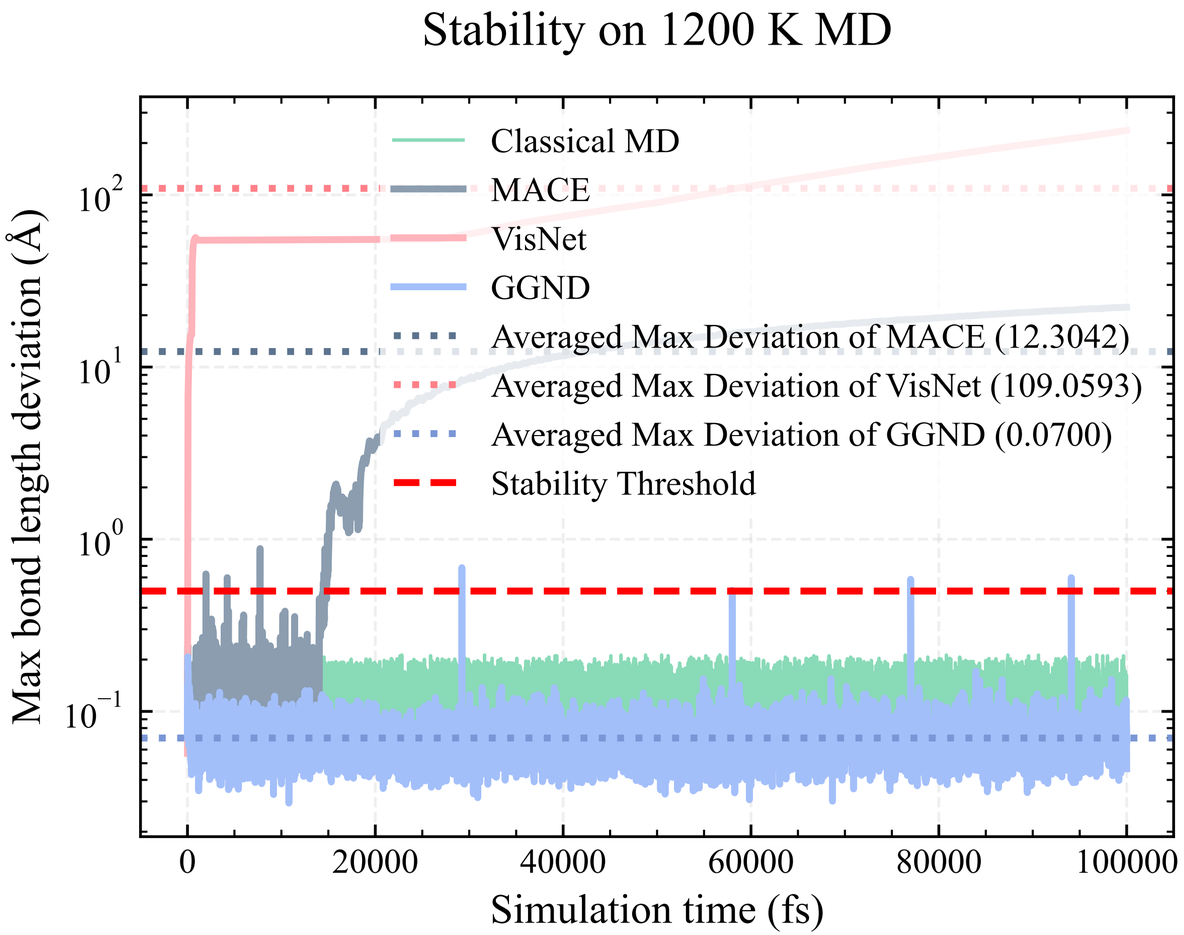


Results: stability breakthrough on 3BPA (small molecule)

Our GGND is plug-and-play, enable stable MD simulations of all baselines up to 29 ps, acquiring an order of magnitude improvement.

Conformation	Metrics	MACE	+GGND	NequIP	+GGND	SEGNO	+GGND	VisNet	+GGND
300K	E (↓)	0.113	**0.010**	0.165	**0.094**	0.593	**0.293**	0.002	0.002
	F (↓)	0.165	**0.022**	0.113	**0.104**	0.359	**0.183**	0.006	0.006
	S (↑)	100	100	100	100	99.812	**100**	100	100
600K	E (↓)	0.161	**0.023**	0.335	**0.122**	0.908	**0.295**	1.405	**0.022**
	F (↓)	0.335	**0.044**	0.161	**0.153**	0.893	**0.193**	0.997	**0.041**
	S (↑)	100	100	98.271	**100**	59.892	**100**	25.358	**100**
1200K	E (↓)	0.271	**0.109**	0.770	**0.477**	2.836	**0.503**	3.464	**0.583**
	F (↓)	0.770	**0.111**	0.271	**0.269**	1.238	**0.285**	1.404	**0.304**
	S (↑)	1.965	**29.218**	0.018	**17.052**	0.009	**16.201**	0.004	**11.209**
Dihedral Slices	E (↓)	0.169	**0.012**	0.387	**0.375**	0.923	**0.267**	0.789	**0.050**
	F (↓)	0.289	**0.017**	0.242	**0.189**	0.795	**0.192**	0.697	**0.039**
	S (↑)	100	100	89.119	**100**	72.282	**100**	47.785	**100**

Results: The averaged max deviation is well-below the threshold compared to baslines



Results: stability breakthrough on SAMD23 (materials)

GGND achieved the best energy and force predictions while obtained the near-perfect ~100 ps stability

Molecule	Splits	Metrics	NequIP	MACE	Allegro	Neural P3M	QuinNet	Equiformer V2	LSRM	FreeCG	GGND
SiN	Test	E/A (↓)	0.013	0.012	0.015	0.010	0.010	0.010	0.010	0.011	**0.009**
		F (↓)	0.598	0.526	0.673	0.485	0.490	0.451	0.490	0.494	**0.443**
		S (↑)	69.009	78.845	63.583	88.280	83.286	98.284	81.000	84.500	**100**
	OOD	E/A (↓)	0.022	0.018	0.028	0.016	0.017	0.021	0.018	0.018	**0.015**
		F (↓)	1.018	0.912	1.185	0.837	0.836	0.972	0.832	0.844	**0.754**
		S (↑)	63.733	65.710	55.824	85.888	86.512	82.031	74.217	76.631	**99.892**
HfO	Test	E/A (↓)	0.007	0.006	0.007	0.006	0.006	**0.005**	0.006	0.006	**0.005**
		F (↓)	0.377	0.335	0.385	0.311	0.304	0.298	0.312	0.315	**0.179**
		S (↑)	65.377	78.054	64.282	90.432	89.034	97.184	87.353	85.040	**100**
	OOD	E/A (↓)	0.011	0.010	0.012	0.009	0.009	0.010	0.010	0.009	**0.008**
		F (↓)	0.430	0.570	0.593	0.459	0.457	0.683	0.544	0.593	**0.279**
		S (↑)	61.621	65.689	60.982	84.209	85.453	79.762	86.373	75.916	**97.928**

Takeaways

- We found that MD instability could be caused by OOD topology shift
- Our proposed GGND, an equivariant global diffusion with local message passing, can achieve stable MD simulations