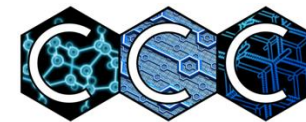
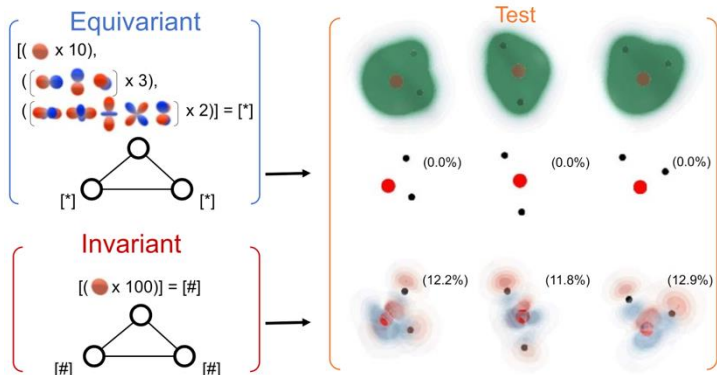


# Breaking the Equivariance

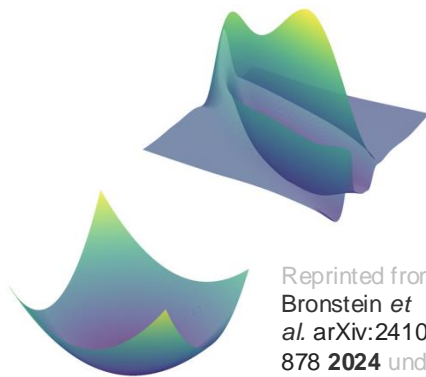


Two models, one invariant and one equivariant, are trained on the electron density of a single water molecule. Both networks are tested on three randomly rotated versions of the input water molecule.



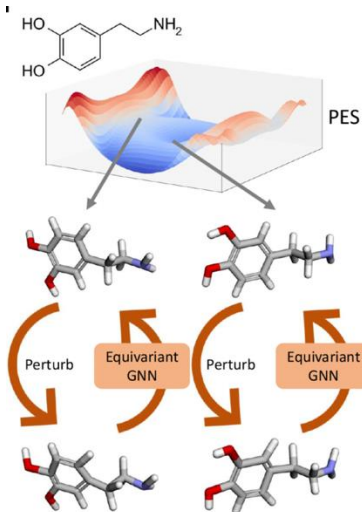
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Loss surface around local minima of trained models on N-body dynamical system.

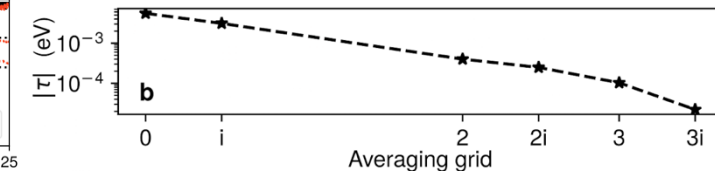
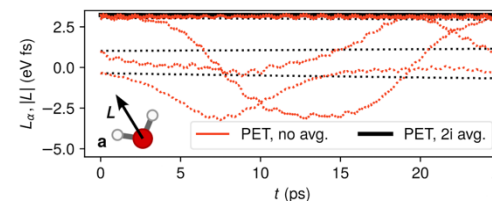
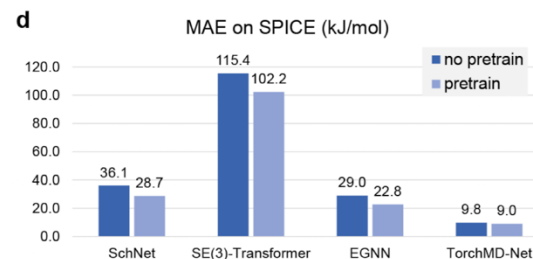
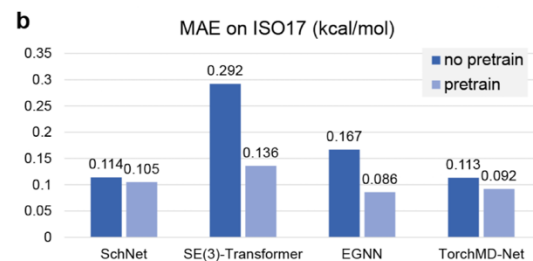


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Training a GNN to match the perturbation noise is equivalent to learning a pseudo force field when assuming the probability of atomic positions around a sampled conformation follows a Gaussian distribution.

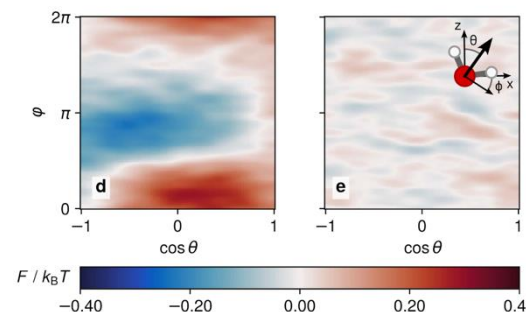


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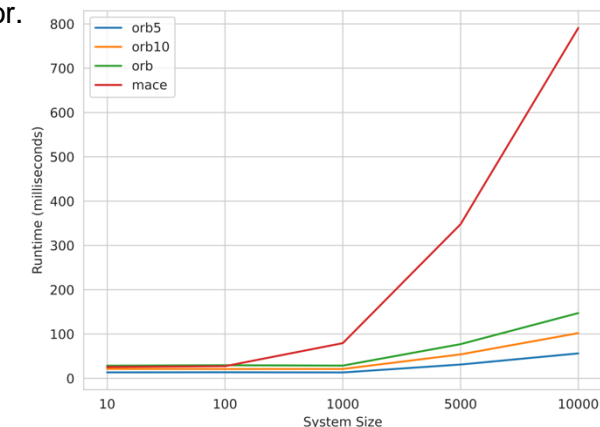
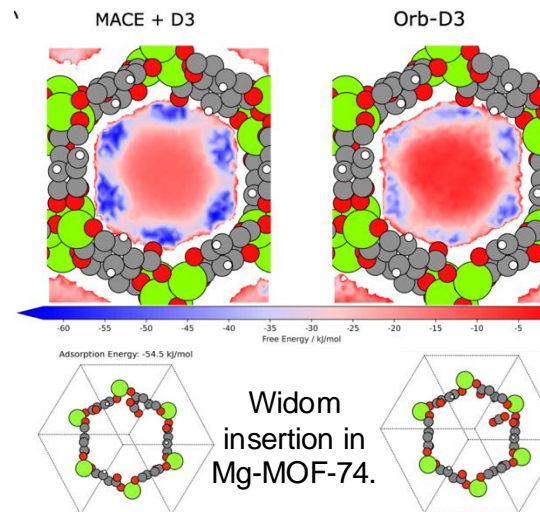
Rotational averaging mitigates symmetry breaking and systematically reduces the magnitude of  $|\tau|$ —which does not eliminate precession, but slows it down dramatically, and effectively eliminates the fluctuations of  $|L|$ .

Oriental free energy for the water molecule computed over a long constant-temperature simulation without (d) and with 2i rotational averaging (e).



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Orb = non-equivariant graph network simulator.



Orb models are 3-6 times faster than existing universal potentials.

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