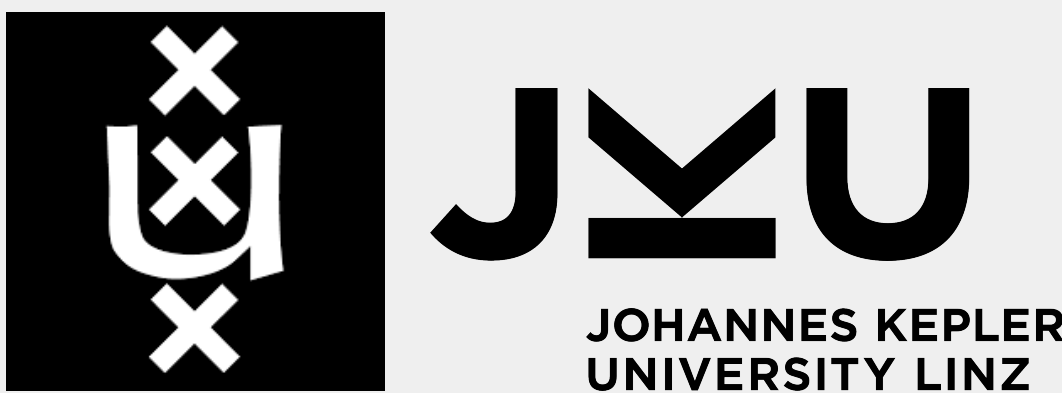


Geometric And Physical Quantities Improve E(3) Equivariant Message Passing

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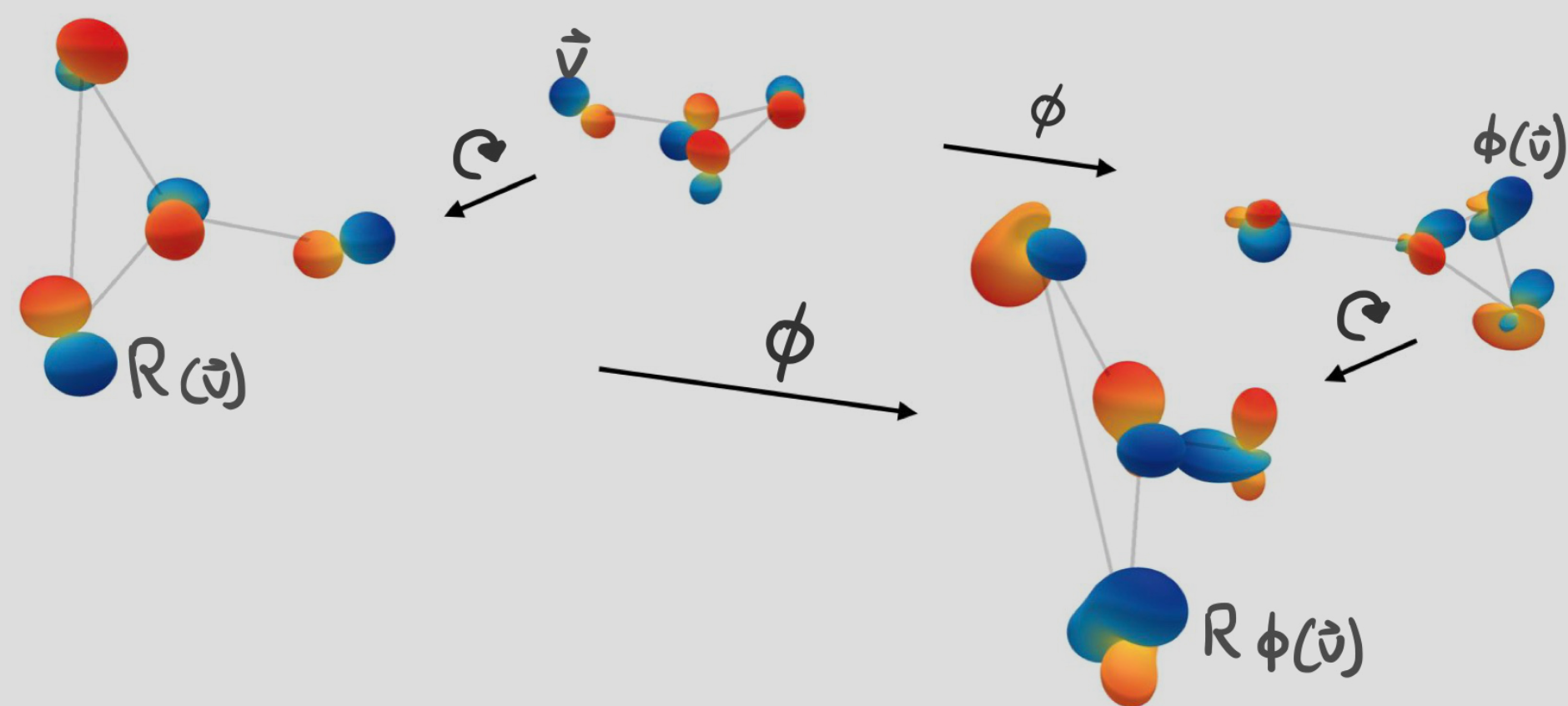
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Vector-valued information

Vector valued quantities are abundant in natural sciences. Let's exploit, embed, or learn geometric/physical cues!

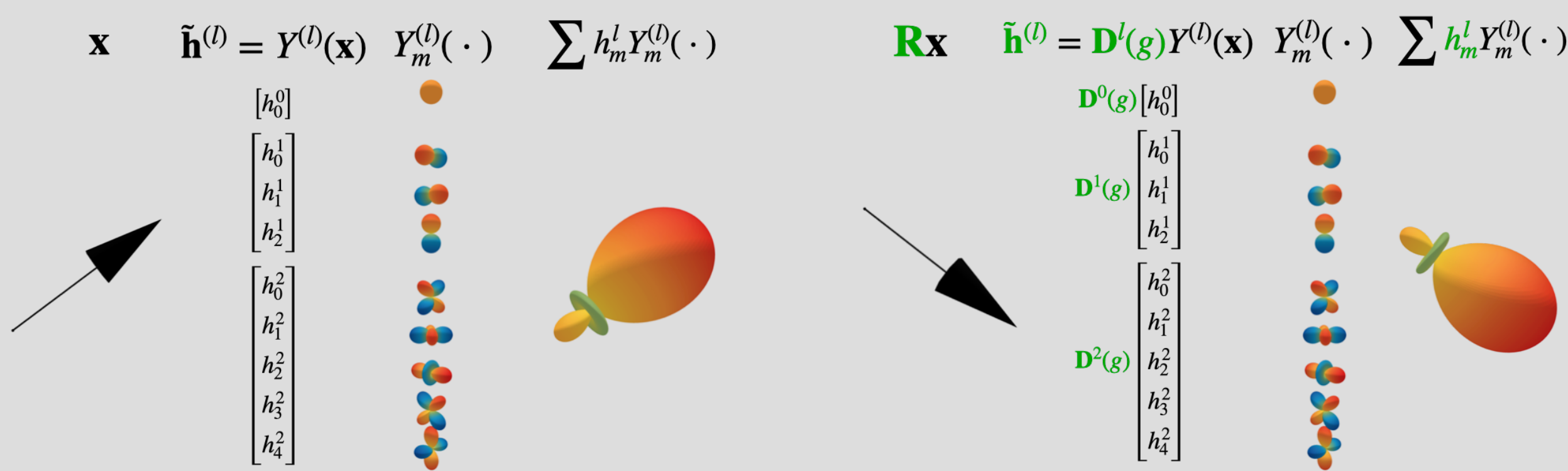
- Extend E(3) equivariance towards vector-valued quantities, e.g. force or velocity.
- E(3) equivariance = equivariance with respect to rotations, translation, reflections, (and permutations).
- Augment message and node update networks with vector-valued quantities.



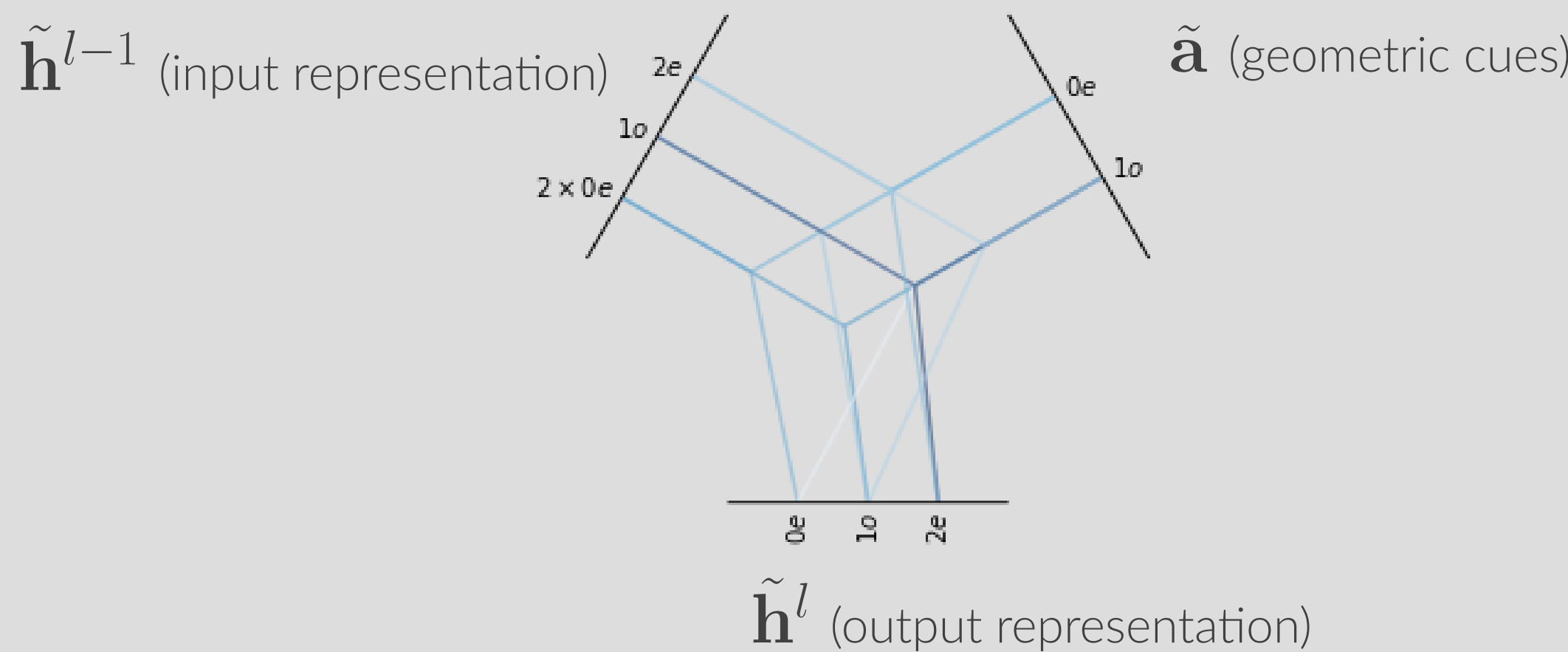
Steerable features, steerable vector spaces, steerable MLPs

Loosely speaking, steerability wrt certain group: objects transform with matrix-vector multiplication.

- We work in the basis spanned by spherical harmonics.
- Spherical harmonics embedding is equivariant w.r.t rotations (we work with subspaces on which rotations act).
- Clebsch-Gordan (CG) tensor product provides equivariant map between steerable vector spaces.



Steerable E(3) Equivariant Graph Neural Networks (SEGNNs)



Message (ϕ_m) and node update (ϕ_f) networks as CG tensor products interleaved with non-linearities:

$$\tilde{\mathbf{m}}_{ij} = \phi_m \left(\underbrace{\tilde{\mathbf{f}}_i, \tilde{\mathbf{f}}_j, \|\mathbf{x}_j - \mathbf{x}_i\|^2}_{\tilde{\mathbf{h}}_{ij}}, \tilde{\mathbf{a}}_{ij} \right); \quad \tilde{\mathbf{f}}'_i = \phi_f \left(\underbrace{\tilde{\mathbf{f}}_i, \sum_{j \in \mathcal{N}(i)} \tilde{\mathbf{m}}_{ij}}_{\tilde{\mathbf{h}}_i}, \tilde{\mathbf{a}}_i \right)$$

Non-linear vs linear convolution

			Task	α	$\Delta\epsilon$	ϵ_{HOMO}	ϵ_{LUMO}	μ	C_v	Table 2: Comparison on QM9.
			Units	bohr ³	meV	meV	meV	D	cal/mol	
non-linear	regular	no geometry	NMP	.092	69	43	38	.030	.040	
		\mathbb{R}^3	SchNet *	.235	63	41	34	.033	.033	
pseudo-linear	steerable	\mathbb{R}^3	Cormorant	.085	61	34	38	.038	.026	
		SE(3)	L1Net	.088	68	46	35	.043	.031	
pseudo-linear	steerable	G	LieConv	.084	49	30	25	.032	.038	
		SE(3)	TFN	.223	58	40	38	.064	.101	
pseudo-linear	steerable	SE(3)	SE(3)-Tr.	.142	53	35	33	.051	.054	
		$\mathbb{R}^3 \times S^2 \times \mathbb{R}^+$	DimeNet++ *	.043	32	24	19	.029	.023	
non-linear	regular	$\mathbb{R}^3 \times S^2 \times \mathbb{R}^+$	SphereNet *	.046	32	23	18	.026	.021	
		SE(3)	PaiNN *	.045	45	27	20	.012	.024	
non-linear	regular	\mathbb{R}^3	EGNN	.071	48	29	25	.029	.031	
		SE(3)	SEGNN (Ours)	.060	42	24	21	.023	.031	

- Group convolutions, **one way** or **the other** (Bekkers 2019):
 - “Any equivariant linear layer between feat maps on **homogeneous spaces** is a group convolution”
 - Steerable** vs **regular** convolution
 - If $X \equiv G/H$: kernel has symmetry constraints (SchNet, EGNN, ...)
 - Idea of **non-linear convolution** discussed in Section 3.
- Recent work by Cesa, Lang & Weiler (2022): comprehensive theory and code framework for general steerable CNNs.

New steerable activation functions

Framing message passing as non-linear convolution allows us to see the node update as **new equivariant activation function**:

$$\tilde{\mathbf{f}}'_i = \phi_f \left(\tilde{\mathbf{f}}_i, \underbrace{\sum_{j \in \mathcal{N}(i)} \tilde{\mathbf{m}}_{ij}}_{\tilde{\mathbf{h}}_i}, \tilde{\mathbf{a}}_i \right).$$

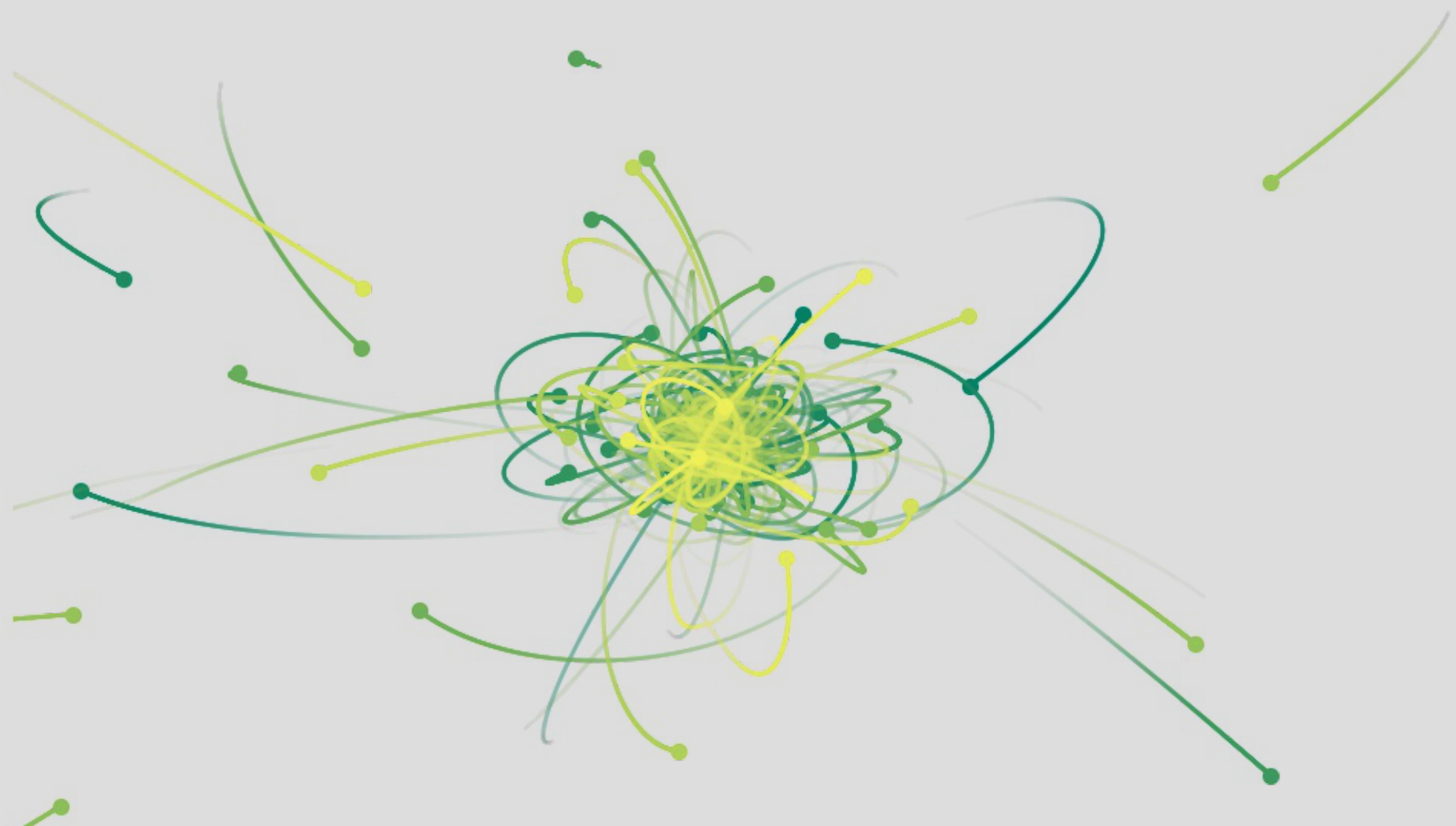
Activation function as non-linear MLPs, which are applied node-wise.

Performance and applicability

SEGNNs work especially well when there is physical and geometrical information available:

- Enrich (steer) node updates via velocity, force, momentum, acceleration, spin, angular momentum ...
- Enrich (steer) messages via relative position, relative forces, dipole moments, ...

Method	MSE
SE(3)-Tr.	.0244
TFN	.0155
NMP	.0107
Radial Field	.0104
EGNN	.0070
SE _{linear}	.0116
SE _{non-linear}	.0060
SEGNN _G	.0056
SEGNN _{G+P}	.0043



References

- [1] Erik J Bekkers. B-spline cnns on lie groups. In *International Conference on Learning Representations*, 2019.
- [2] Mario Geiger, Tess Smidt, Alby M., Benjamin Kurt Miller, Wouter Boomsma, Bradley Dice, Kostiantyn Lapchevskyi, Maurice Weiler, Michat Tyszkiewicz, Simon Batzner, Jes Frellsen, Nuri Jung, Sophia Sanborn, Josh Rackers, and Michael Bailey. e3nn/e3nn: 2021-04-21, April 2021.