

Table 1: The detailed prediction error ($\times 10^{-2}$) w.r.t. k , average of 3 runs.

Base Model	N-body (1,2,0)				MD17 (Aspirin)							
	k=0	k=1	k=2	k=5	k=0	k=1	k=2	k=3	k=4	k=5	k=6	k=8
RF	3.5	3.07	2.84	2.79	10.94	10.91	10.87	10.87	10.87	10.86	10.86	10.86
EGNN	2.81	2.57	2.41	2.40	14.41	9.65	9.63	9.65	9.62	9.60	9.52	9.49
GMN	1.84	1.59	1.55	1.55	10.14	9.72	9.50	9.51	9.34	9.29	9.51	9.49

Table 2: A comparison between NC and NC (coefficients = 1).

Method	N-body (1,2,0)		MD17 (Aspirin)		Motion	
	Intermediate Vel. Error	Final Error	Intermediate Vel. Error	Final Error	Intermediate Vel. Error	Final Error
GMN	-	1.84	-	10.14	-	43.9
NC (coefficients = 1)	22.79	1.78	100.50	9.64	182.20	48.4
NC	4.33	1.55	6.37	9.50	3.27	30.0
NC ⁺ (coefficients = 1)	13.27	1.81	10.53	9.91	80.89	153.6
NC ⁺	1.41	1.57	0.73	9.40	0.24	29.6

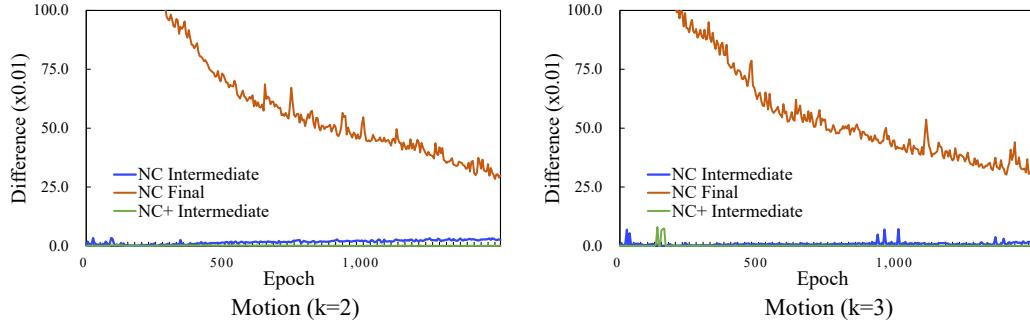


Figure 1: The final error of NC, the intermediate velocity error of NC, and the intermediate velocity error of NC⁺ on the valid set of the Motion dataset, w.r.t. training epoch.

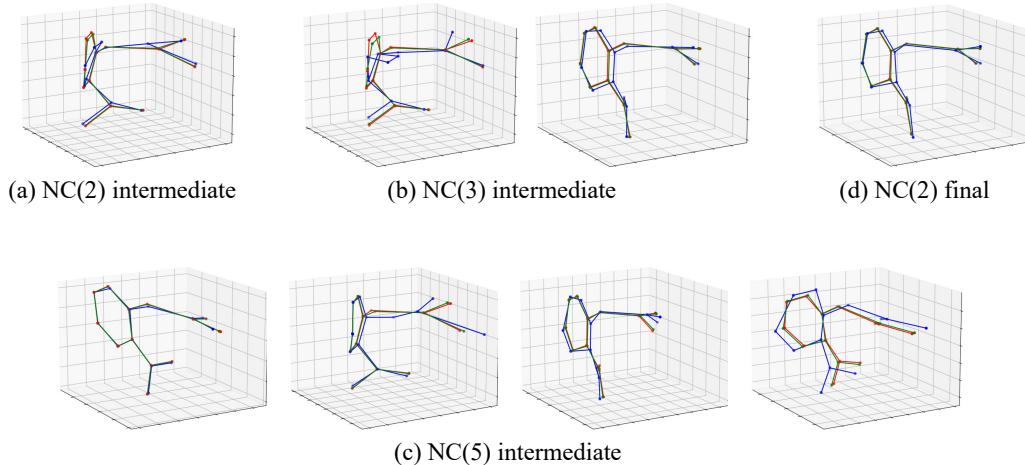


Figure 2: MD17 (Aspirin) Visualization of the intermediate velocities w.r.t. k . The red, blue, and green lines denote the target, prediction of NC, and prediction of NC⁺, respectively.