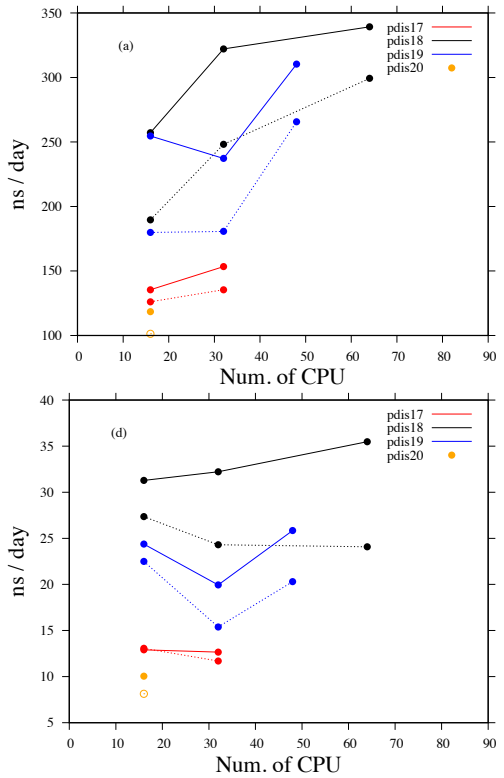
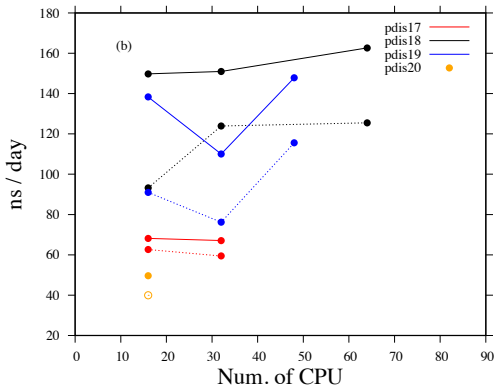
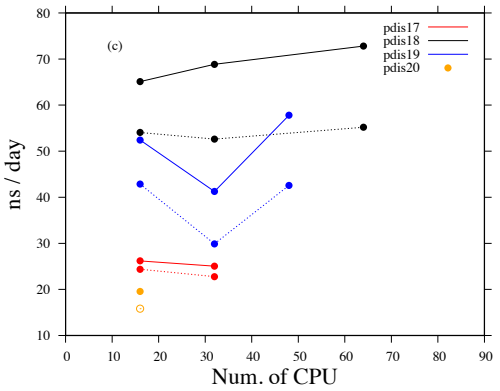
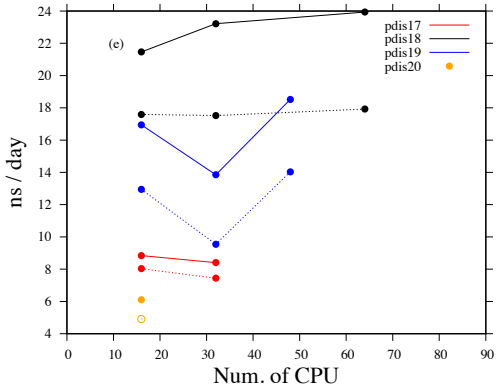
Benchmark of gromacs on PDIS









Solid-line: gromacs-2022
Dashed-line: gromacs-2018

(a) Chignolin in water(14,948 atoms), dt=2fs
(b) Lysozyme in water(35,984 atoms), dt=2fs
(c) SAM50-TOM40 in hydrated-membrane(149,052 atoms), dt=4fs(HMR)
(d) SAM50-TOM40 in hydrated-membrane(154,885 atoms), dt=2fs
(e) Protein+DNA in water(274,917 atoms), dt=2fs

		DockQ/iRMS/LRMS	DockQ/iRMS/LRMS/iPTM	DockQ/iRMS/LRMS/iPTM
ID CASP14(PDB)	Stoio.	Folddock	Alphafold-multimer(v-2.1.1)	Alphafold-multimer(v-2.2.0)
T1032(6N64)	A2	0.493/4.877/6.925	0.471/4.980/7.352/0.712	0.450/5.111/7.696/0.688
H1036(6VN1)	A3B3C3		-	-
T1038(6YA2)	A2		0.928/0.504/2.232/0.840	0.954/0.418/1.937/0.852
H1045(6XOD)	AB	0.024/8.600/40.855		
H1046(6PX4)	AB	0.737/1.430/2.667	0.776/1.344/1.805/0.903	0.760/1.423/2.181/0.903
T1054(6V4V)	A2	0.027/17.858/29.814	0.015/19.521/42.029/0.625	0.033/13.538/29.545/0.242
H1065(7M5F)	AB	0.017/16.573/40.516	0.878/0.878/1.118/0.913	0.889/0.842/0.919/0.889
H1072(6R17)	A2B2			0.760/1.599/1.785/0.784 (AB vs AB) 0.759/1.607/1.974/0.774 (AA vs BB)
T1073	A4			
T1078(7CWP)	A2	0.787/1.022/1.448	0.046/16.381/25.319/0.563	0.517/2.236/2.710/0.777
T1080	A3			

0.00 <= DockQ < 0.23 - Incorrect
0.23 <= DockQ < 0.49 - Acceptable quality
0.49 <= DockQ < 0.80 - Medium quality
DockQ >= 0.80 - High quality