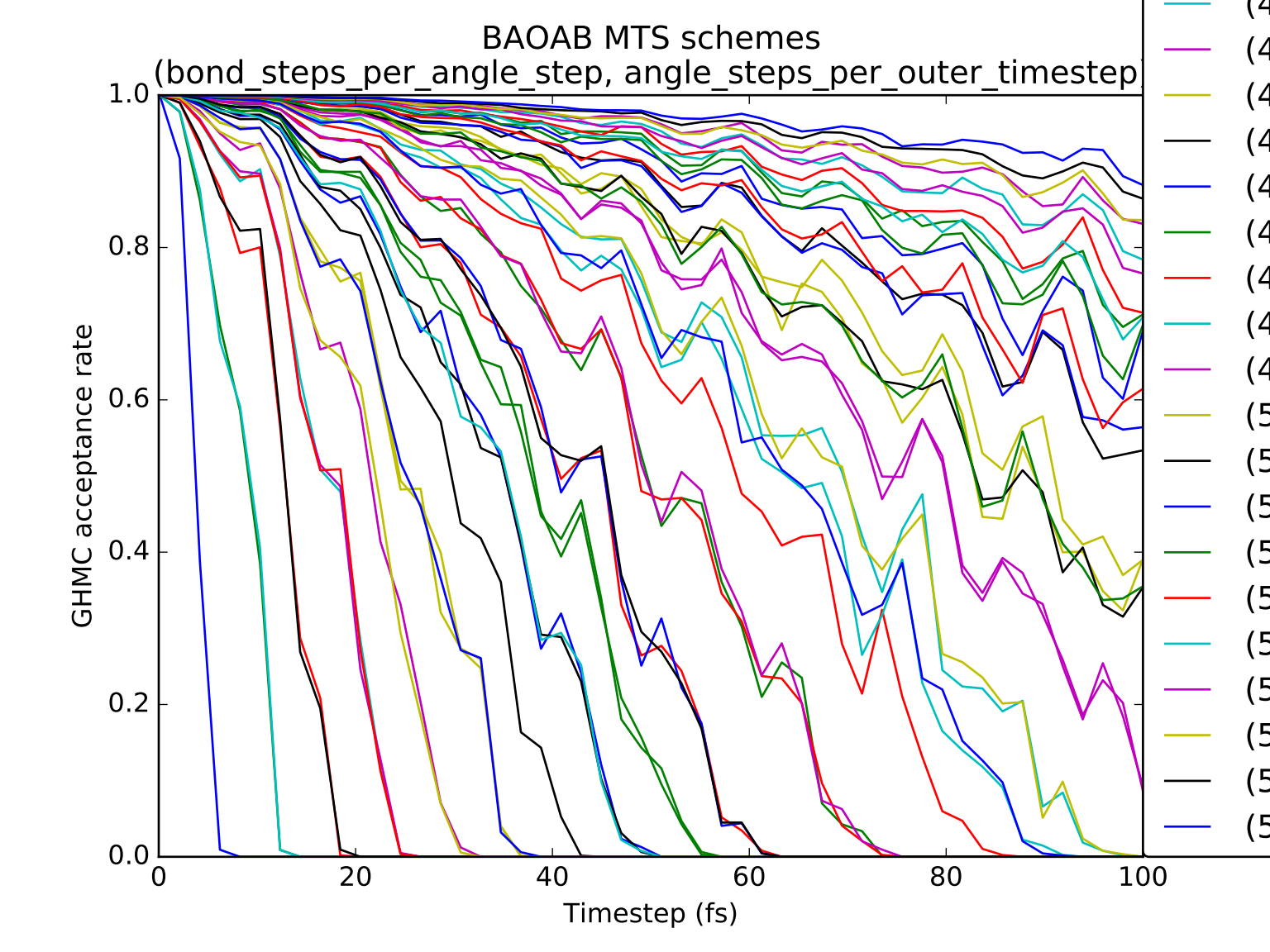
BAOAB MTS schemes
(bond_steps_per_angle_step, angle_steps_per_outer_timestep)
GHMC acceptance rate
Timestep (fs)
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80
100