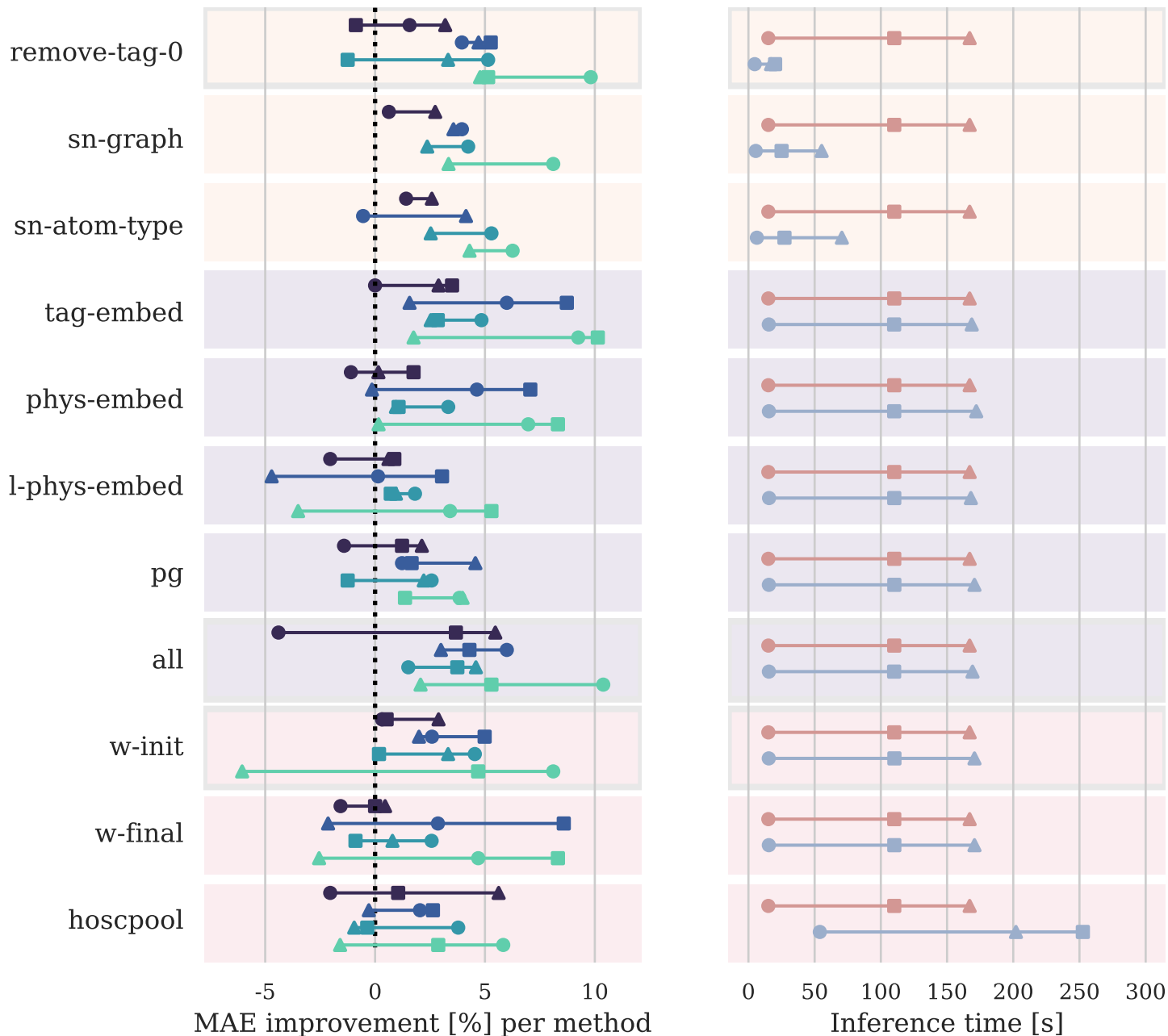


ID
 OOD-ad
 OOD-cat
 OOD-both
 SchNet
 D++
 ForceNet

Baseline
 PhAST



Graph creation

Atom embed.

Energy head