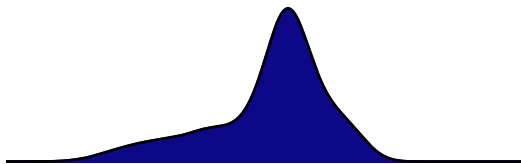


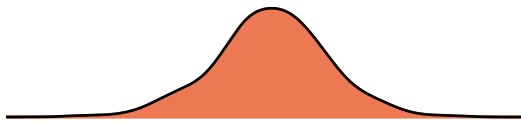
Empirical



Physical (MM)



Physical (QM)



-5                      0                      5  
 $\Delta \log P$  error (calc - exp)