

Just run naïve dynamics?

Angular resolution in space \Rightarrow Time resolution $\sim f_s$

Events of interest: $\sim 1/\text{ms}$; on average 10^{12} time steps

Modern computers: 10^8 time steps (100ns) per day!

10^4 days (~ 30 years) ... for one event!

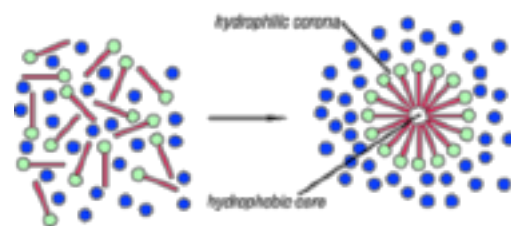
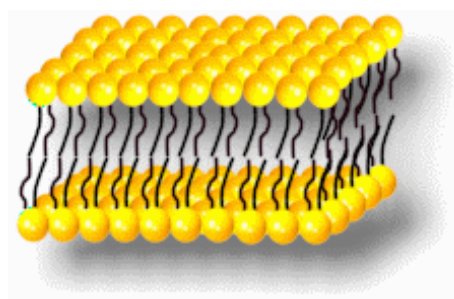
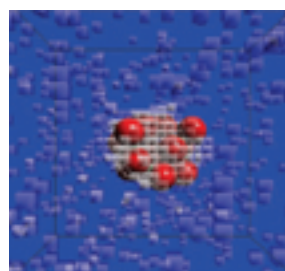
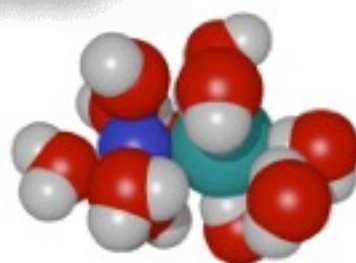
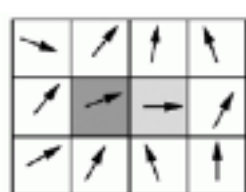
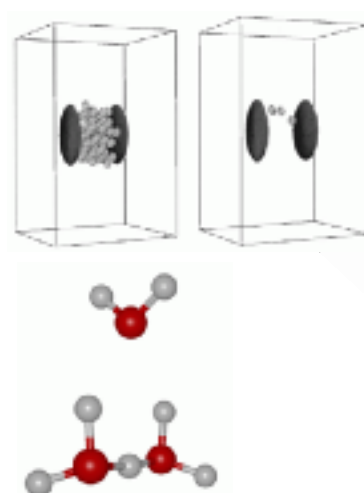
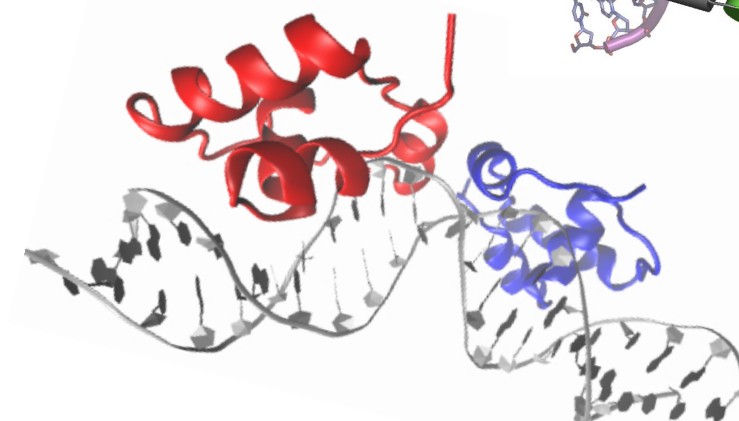
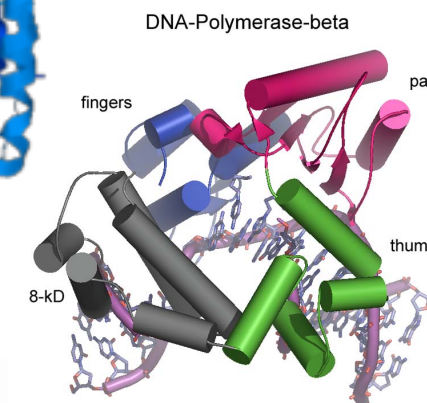
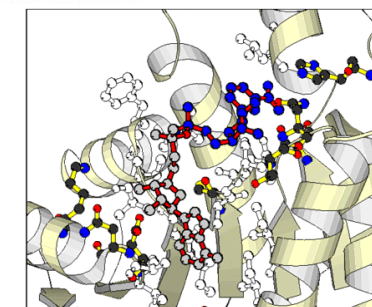
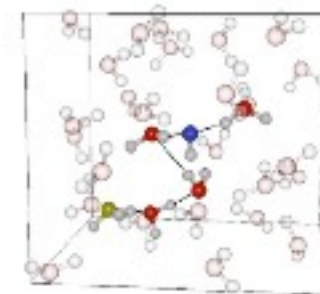
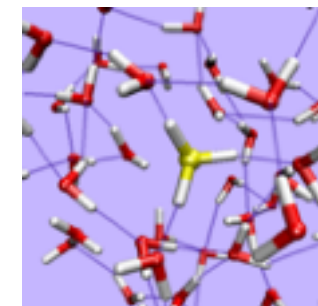
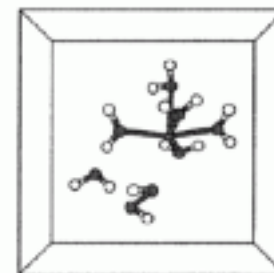
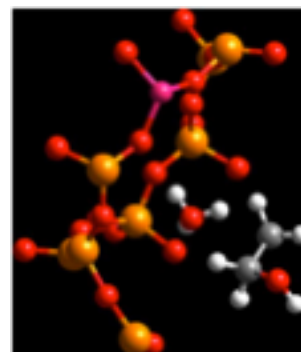
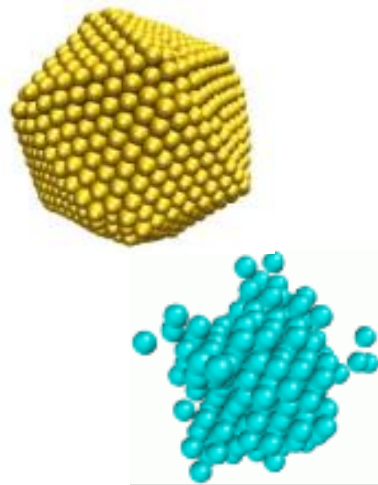
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Atomistic resolution in space \implies Time resolution \sim fs

Events of interest: \sim 1/ms; on average 10^{12} time steps

Modern computers: 10^8 time steps (100 ns) per day!

10^4 days (\sim 30 years) ... for **one** event!



crystallization & self-assembly

catalysis

reactions

enzyme reactions

folding & binding

RARE EVENTS