Just run naïve dynamics?

Atomistic resolution in space $\implies$ Time resolution $\sim$ fs

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

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RARE EVENTS

crystallization & self-assembly

catalysis

reactions

complex fluids

enzyme reactions

solvent effects

conformational changes

folding & binding

DNA-Polymerase-beta

fingers

palm

thumb

8-kD