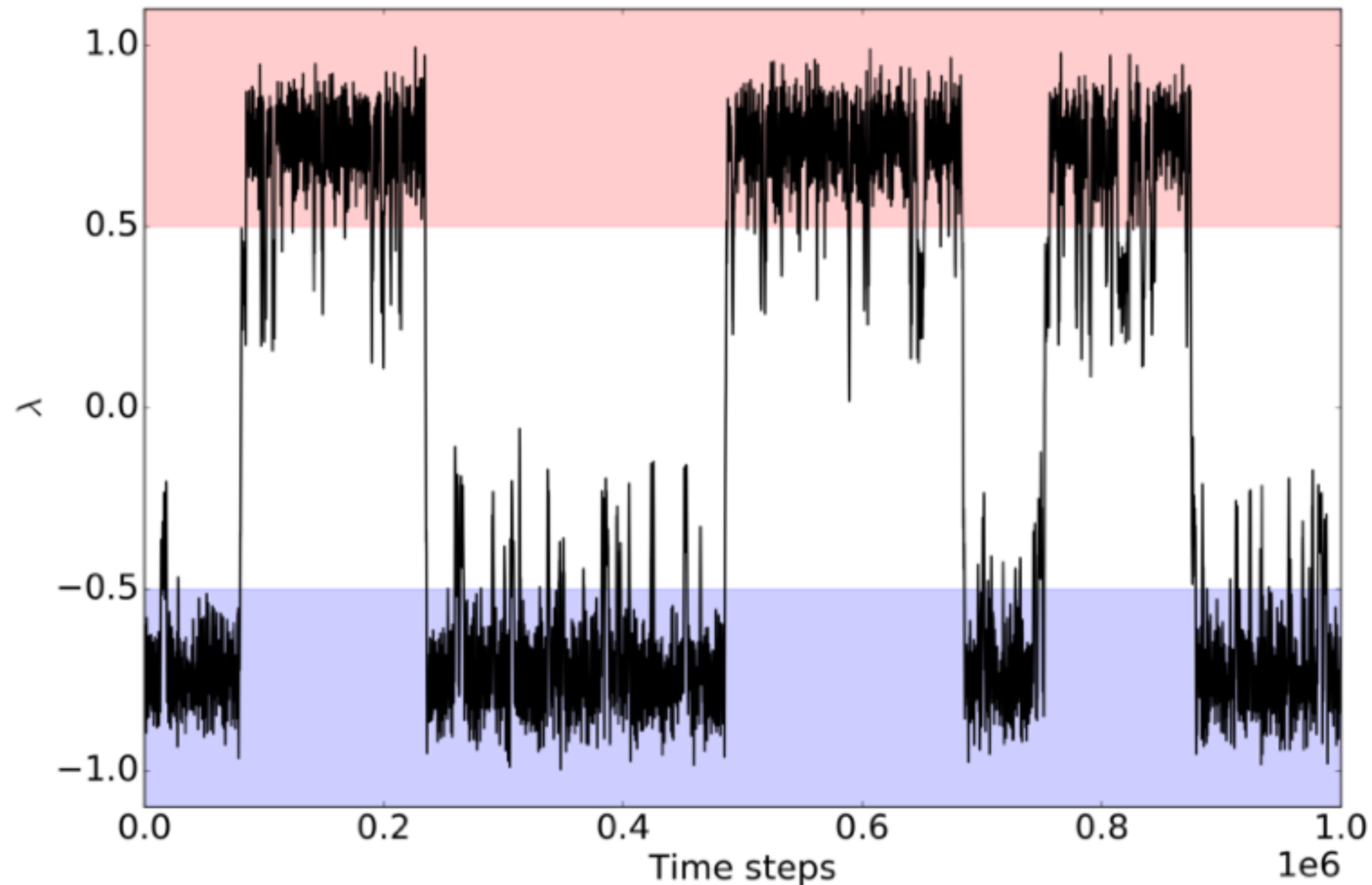


Simulation philosophy

- ***Unbiased dynamics:*** Make as few assumptions as possible about what degrees of freedom are important
- ***Full atomistic:*** High resolution in space and time
- ***Calculate rates, observe mechanisms:***
Compare with experiment and provide new insight

Just run naïve dynamics?



Separation of time scales:
fundamental time scale vs. frequency of event