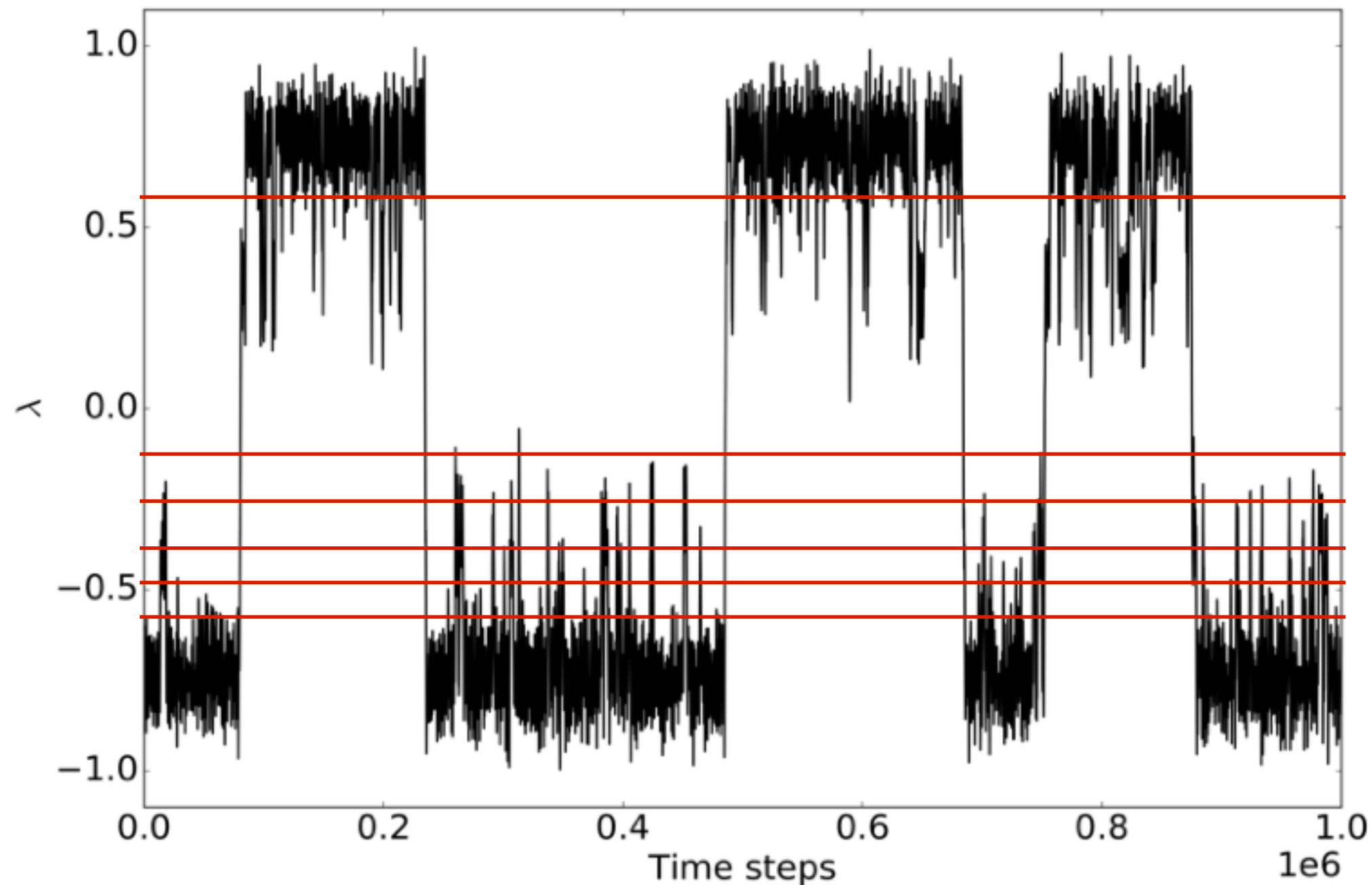


Calculating the rate with TIS

Successive crossing probabilities: multiply a number
~0.1 a bunch of times to get a very small probability

van Erp, Morini, Bolhuis. JCR 118, 7762 (2003).

Calculating the rate with TIS



Successive crossing probabilities: multiply a number ~ 0.1 a bunch of times to get a very small probability

Methods Overview

Transition Path Sampling (TPS)	mechanisms (most of this talk)
Transition Interface Sampling (TIS)	rates free energies (more expensive!)

Variants of both exist to study multiple state systems