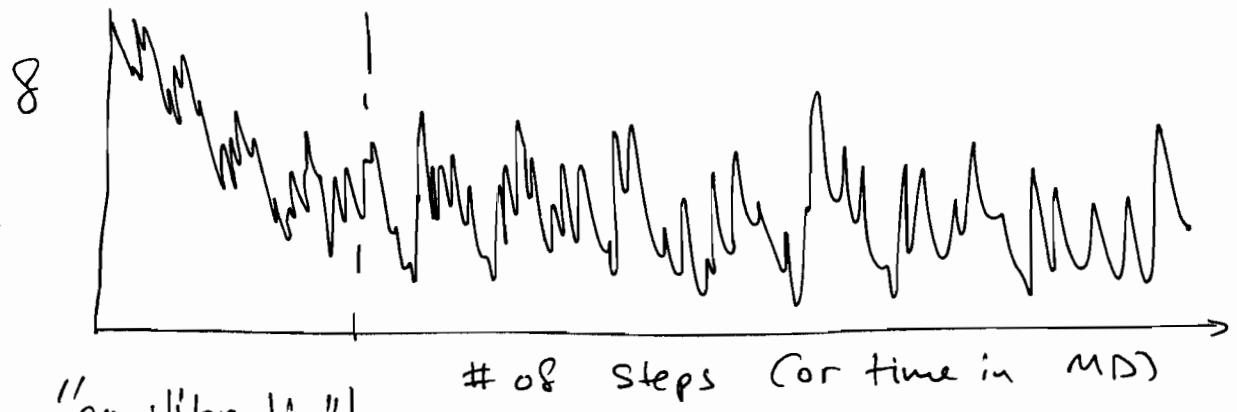
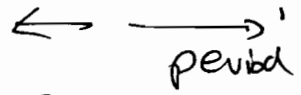


Typical observations in a simulation

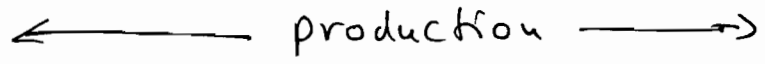


"equilibration"



affected by initial state - discards

# of steps (or time in MD)



production

$$\langle \delta \rangle = \frac{\sum \delta_v}{\# \text{ of production steps}}$$

$$\langle (\delta \delta^2) \rangle = \langle (\delta - \langle \delta \rangle)^2 \rangle$$

is a thermodynamic quantity

e.g.  $\langle (\delta u)^2 \rangle = k_B T \underbrace{C_v}_{\text{heat capacity}}$

To estimate statistical simulation uncertainties, need multiple independent samples; for  $n$  such samples, recall discussion on sampling; need to compute the standard deviation of the  $n$  samples, divide by  $\sqrt{n}$  to get the expected std. deviation from true mean, then multiply by 2 (95% confidence) or 3 (99%).

National brand