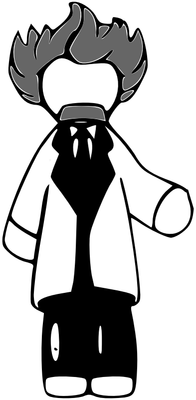
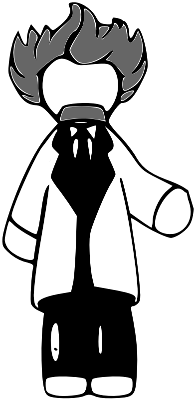
Tau-leaping

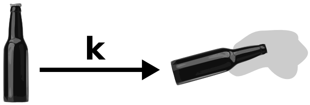
Christian Diener

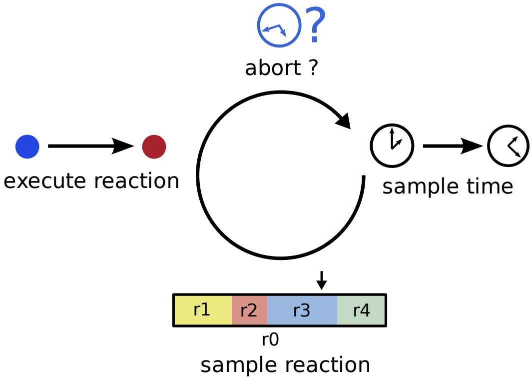
Theoretical Biophysics
Humboldt University of Berlin
Invalidenstraße 42
10115 Berlin

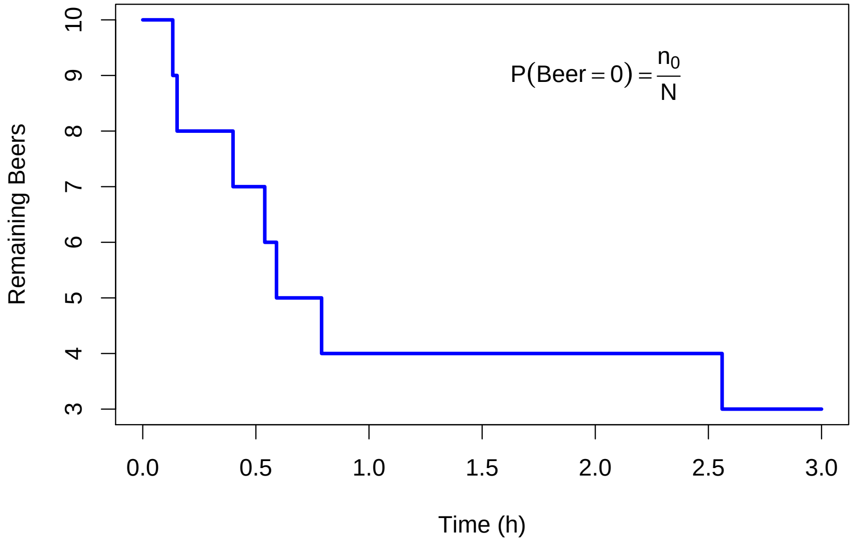
February 8th, 2010



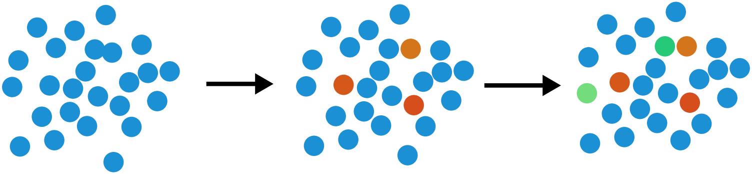



k


?
abort ?
execute reaction
sample time
r1
r2
r3
r4
r0
sample reaction


$P(\text{Beer}=0)=\frac{n_0}{N}$
Remaining Beers
Time (h)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3
4
5
6
7
8
9
10

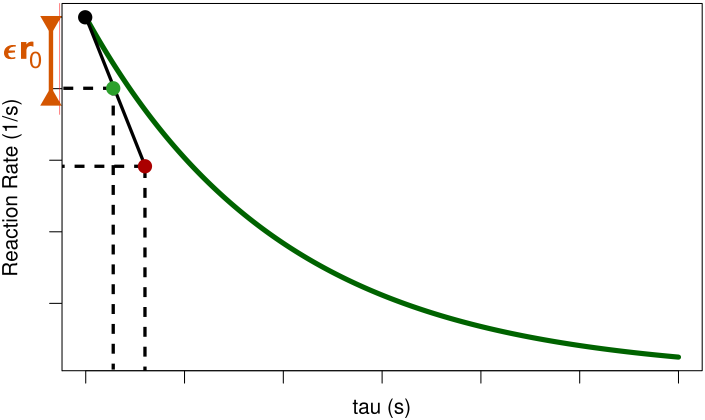
slow slow slow slow slow slow slow slow slow



Tau-leap

If the propensities are close to being constant we can update the system by

$$\mathbf{S}(t+\tau) = \mathbf{S}(t) + \sum_j \rho_j \cdot \phi_j$$



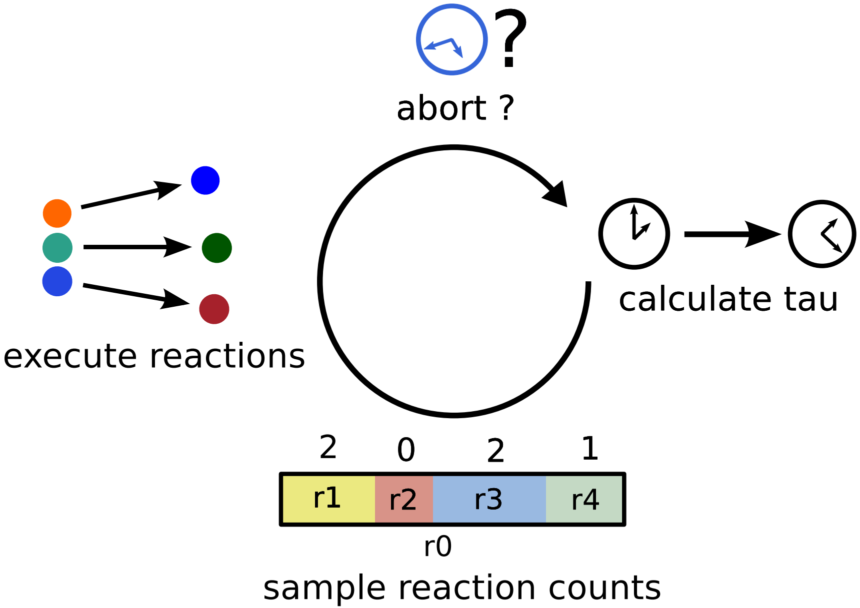
$$\forall j : \langle \Delta r_j(\mathbf{S}, \tau) \rangle \leq \epsilon \cdot r_0(\mathbf{S}, t) \text{ and } \mathrm{Var}(\Delta r_j(\mathbf{S}, \tau)) \leq \epsilon^2 \cdot r_0(\mathbf{S}, t)^2$$

$$\left\langle \Delta r_j(\mathbf{S},\tau)\right\rangle \approx \sum_l \mathcal{D}_{jl} \cdot r_j(\mathbf{S},t)\tau$$

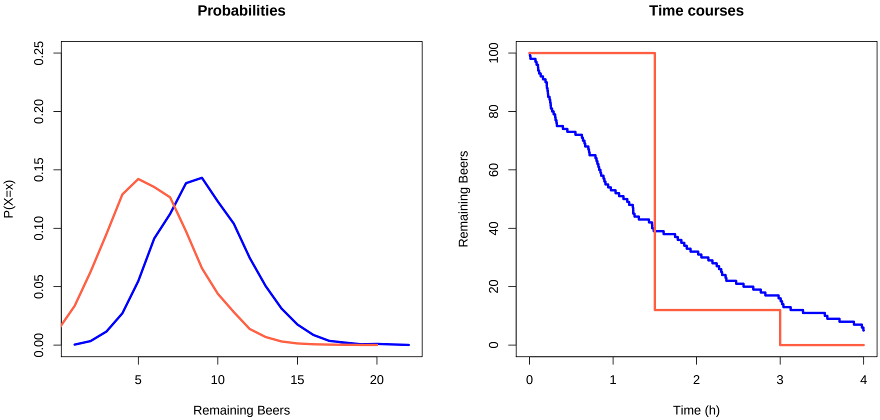
$$\mathrm{Var}\left(\Delta r_j(\mathbf{S},\tau)\right) \approx \sum_l \mathcal{D}_{jl}^2 \cdot r_j(\mathbf{S},t)\tau$$

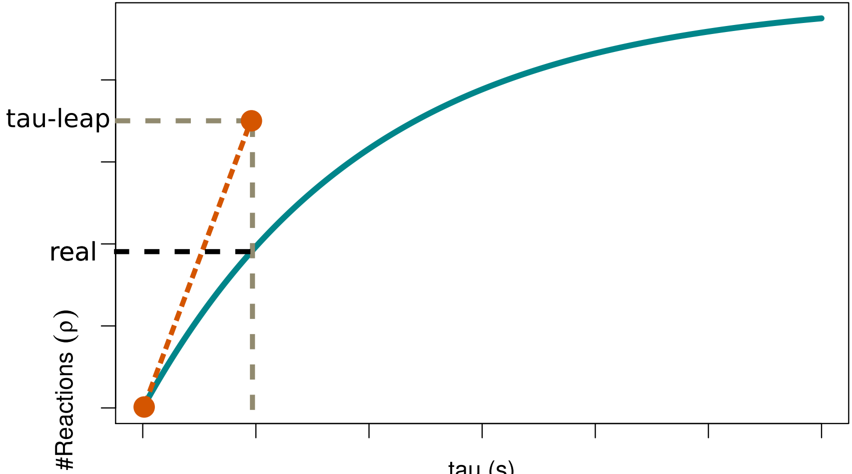
$$\text{“State change”: } \mathcal{D}_{jl} := \sum_k \frac{\partial r_j(\mathbf{S},t)}{\partial S_k} \cdot \phi_{kl}.$$

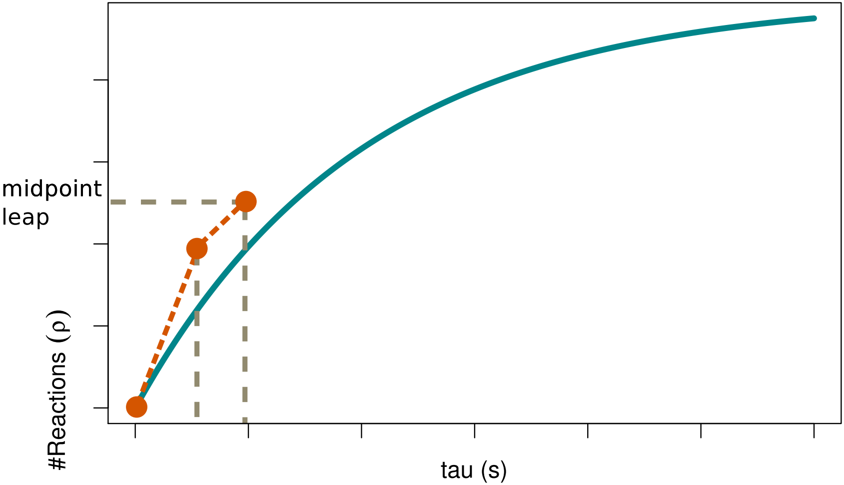
$$\tau = \min_j \left\{ \frac{\epsilon \cdot r_j(\mathbf{S},t)}{\left|\sum_l \mathcal{D}_{jl} \cdot r_j(\mathbf{S},t)\right|}, \frac{\epsilon^2 \cdot r_j(\mathbf{S},t)^2}{\sum_l \mathcal{D}_{jl}^2 \cdot r_j(\mathbf{S},t)} \right\}$$

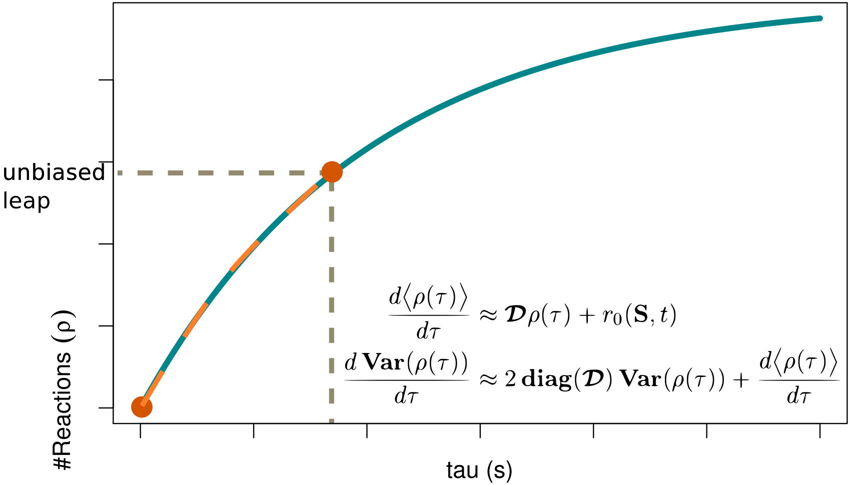

?
abort ?
execute reactions
calculate tau
2 0 2 1
r1 r2 r3 r4
r0
sample reaction counts

What the ... ?!

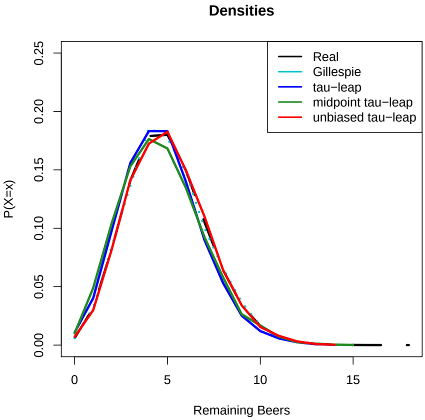

Probabilities
P(X=x)
0.00
0.05
0.10
0.15
0.20
0.25
5
10
15
20
Remaining Beers
Time courses
Remaining Beers
0
20
40
60
80
100
0
1
2
3
4
Time (h)

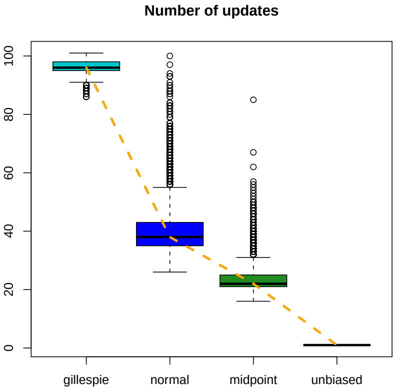

tau-leap
real
#Reactions (ρ)
tau (s)

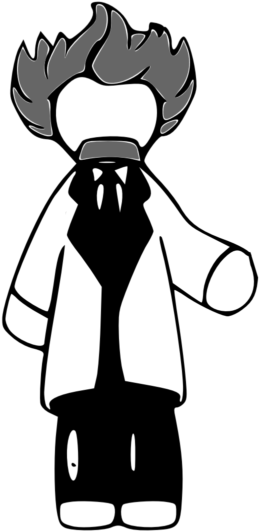

midpoint
leap
#Reactions (ρ)
tau (s)


unbiased
leap
#Reactions (ρ)
tau (s)
$\frac{d\langle\rho(\tau)\rangle}{d\tau} \approx \boldsymbol{\mathcal{D}}\rho(\tau) + r_0(\mathbf{S}, t)$
$\frac{d\,\mathbf{Var}(\rho(\tau))}{d\tau} \approx 2\,\mathbf{diag}(\boldsymbol{\mathcal{D}})\,\mathbf{Var}(\rho(\tau)) + \frac{d\langle\rho(\tau)\rangle}{d\tau}$

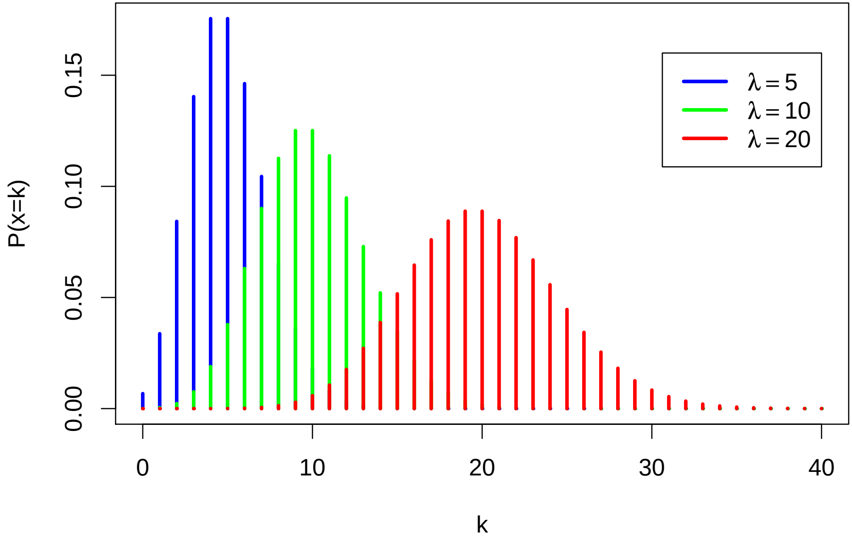
How much faster is it?

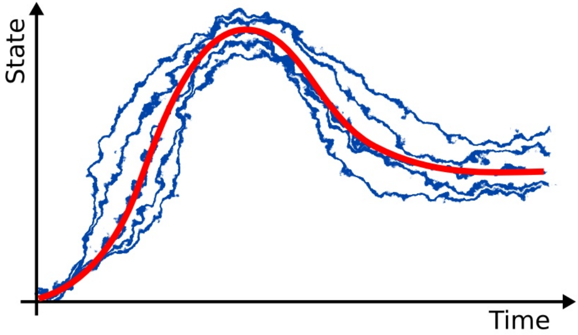




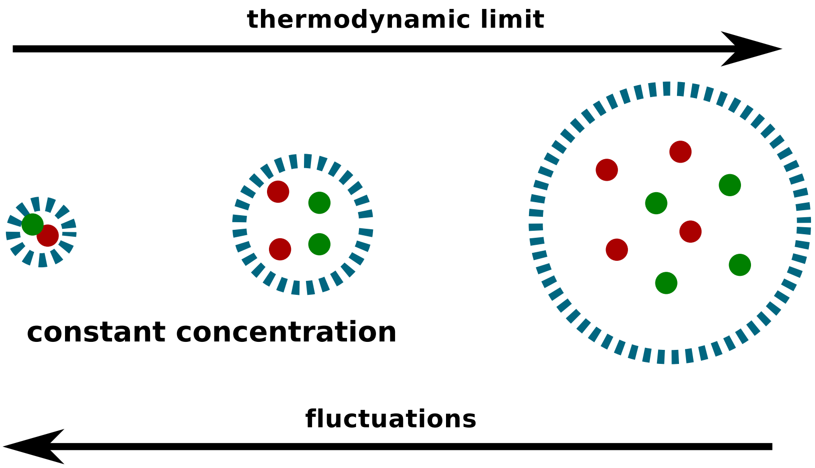


It's getting normal...

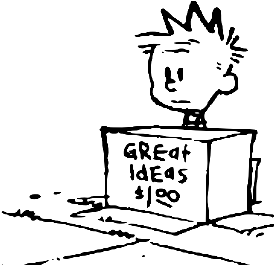




$$\frac{d\mathbf{S}(t)}{dt} = \sum_j \phi_j \cdot r_j(\mathbf{S}, t) + \sum_j \phi_j \cdot \sqrt{r_j(\mathbf{S}, t)} \cdot \Gamma_j(t)$$


thermodynamic limit
constant concentration
fluctuations

Thank you!



International
Max Planck Research School
for Computational Biology
and Scientific Computing