Tuning molecular potential models by imposing kinetic constraints with path reweighting

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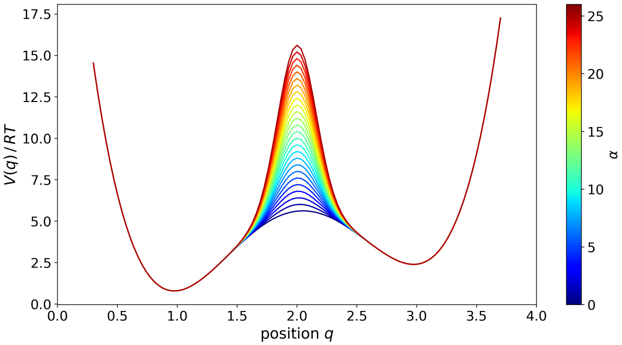
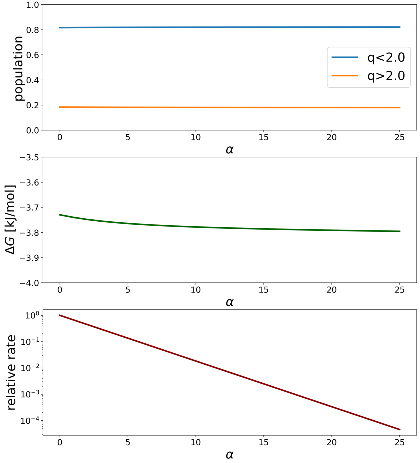
Rare Events: Analysis, Numerics, and Applications
Brin Mathematics Research Center
University of Maryland, USA
Feb 28 - Mar 3, 2023

Dynamic properties of force fields

FF are parametrized against thermodynamic data and are insensitive to barrier heights

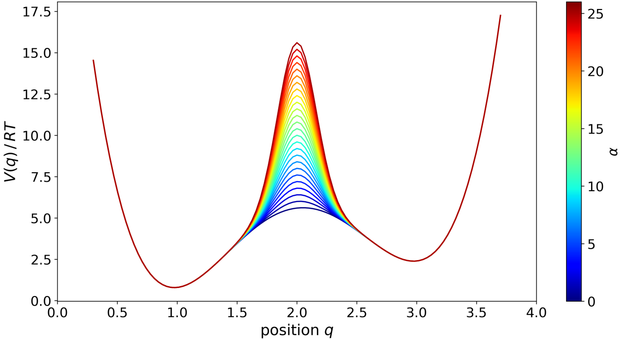


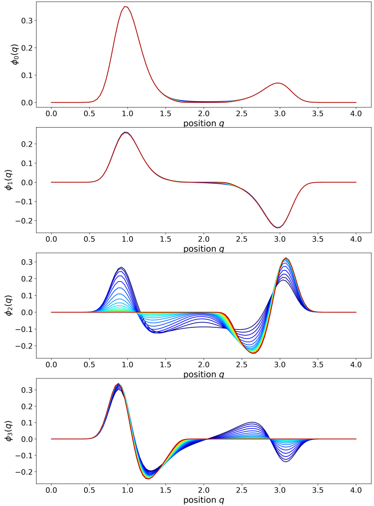


$$Q = \int \exp\left(-\frac{1}{RT} V(q)\right) \, \mathrm{d}q$$

$V(q) = \left[10 \cdot ((q-2)^2 - 1)^2 + \alpha \cdot \exp(-20 \cdot (q-2)^2) + 3q\right]$ kJ/mol and $RT = 2.5$ kJ/mol

Kinetik exchange processes are represented poorly





$$Q = \int \exp\left(-\frac{1}{RT} V(q)\right) \, \mathrm{d}q$$

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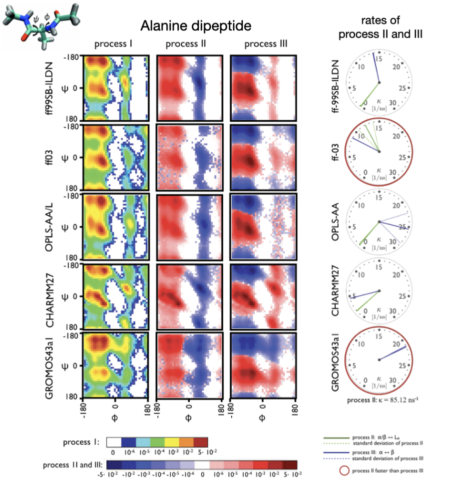
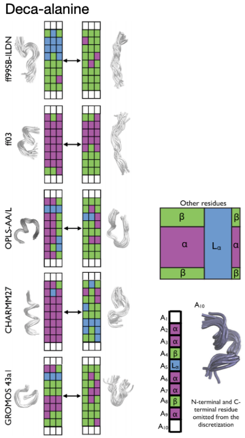
FF with similar thermodynamic properties yield different kinetics





Alanine dipeptide

- dynamics processes consistent across force fields
- rates not consistent across force fields

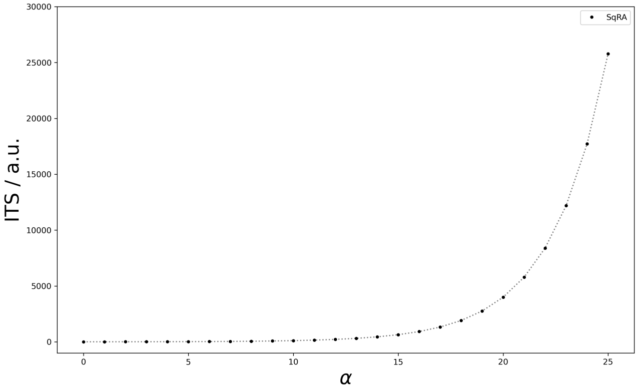
Deca-alanine

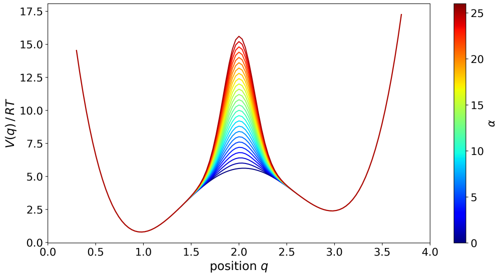
- dynamics processes not consistent across force fields
- rates not consistent across force fields

F Vitalini, AS Mey, F Noé, **BGK** *J. Chem. Phys.* 2015;142(8):02B611.

Path reweighting

Exploring the parameter space by direct sampling has a prohibitive computational cost



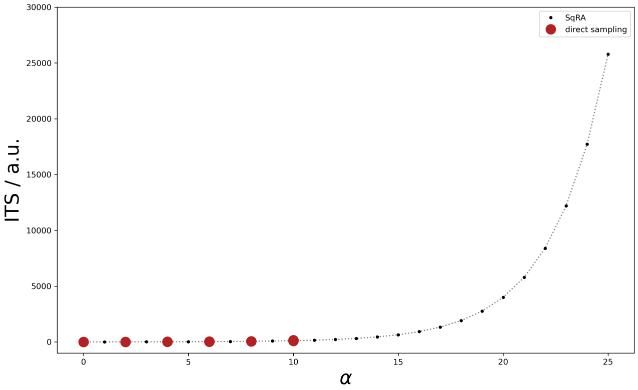


$$V(q) = \left[10 \cdot ((q-2)^2 - 1)^2 + \alpha \cdot \exp(-20 \cdot (q-2)^2) + 3q\right] \text{ kJ/mol}$$

with $RT = 2.5\,\text{kJ/mol}$

Square-root approximation (SqRA) of the Fokker-Planck equation: DJ Bicout, A Szabo (1998), HC Lie, K Fackeldey, M Weber (2018), M Heida (2018)
L Donati, M Heida, **BGK**, M Weber *J. Phys.: Condens. Matter* **2018** *30*, 425201. L Donati, M Weber, **BGK** *J. Phys.: Condens. Matter* **2021** *33*, 115902.

Exploring the parameter space by direct sampling has a prohibitive computational cost



Time-lagged correlation function for a specific parameter value α

$$C_{ij}(\tau,\alpha) = \int_{\Omega_\tau} \mathcal{D}\mathbf{x}\, \chi_i[\mathbf{x}_0] P^{(\alpha)}[\mathbf{x}] \chi_j[\mathbf{x}_\tau]$$

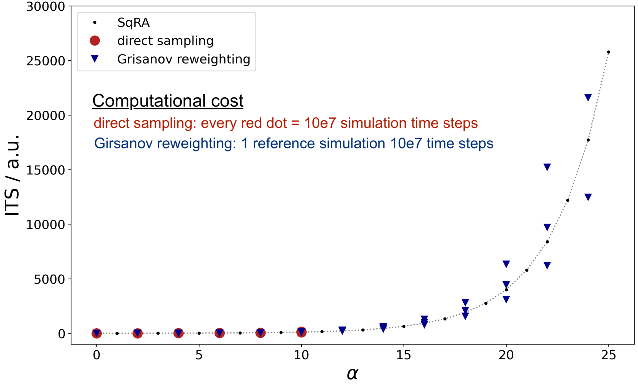
can be estimated from paths simulated at $V + U(\alpha)$

$$\hat{C}_{ij}(\tau,\alpha) = \frac{1}{N_{\mathrm{paths}}} \sum_{k=1}^{N_{\mathrm{paths}}} \chi_i(\mathbf{x}_{k,0}^{(\alpha)}) \chi_j(\mathbf{x}_{k,n}^{(\alpha)})$$

where $\tau = n\Delta t$, and Δt is the integration simulation time step.

$V(q) = \left[10 \cdot ((q-2)^2 - 1)^2 + \alpha \cdot \exp(-20 \cdot (q-2)^2) + 3q\right]$ kJ/mol with $RT = 2.5\,$kJ/mol

Exploring the parameter space by Girsanov reweighting works for low-dim. parameter spaces



Time-lagged correlation function for a specific parameter value α

$$C_{ij}(\tau,\alpha) = \int_{\Omega_\tau} \mathcal{D}\mathbf{x}\, \chi_i[\mathbf{x}_0]\, \frac{Z}{Z(\alpha)} W[\mathbf{x},\alpha] P^{(\alpha=0)}[\mathbf{x}]\chi_j[\mathbf{x}_\tau]$$

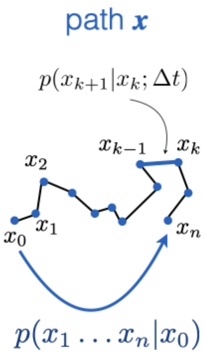
can be estimated by reweighting paths simulated at $V + U(\alpha = 0)$

$$\hat{C}_{ij}(\tau,\alpha) = \frac{1}{N_{\text{paths}}} \sum_{k=1}^{N_{\text{paths}}} \chi_i(\mathbf{x}_{k,0}^{(\alpha=0)})\, \frac{Z}{Z(\alpha)} W[\mathbf{x},\alpha] \chi_j(\mathbf{x}_{k,n}^{(\alpha=0)})$$

$\frac{Z}{Z(\alpha)} W[\mathbf{x},\alpha]$ is the path reweighting factor.

$V(q) = \left[10 \cdot ((q-2)^2 - 1)^2 + \alpha \cdot \exp(-20 \cdot (q-2)^2) + 3q\right]$ kJ/mol with $RT = 2.5$ kJ/mol

Path reweighting for overdamped Langevin



Time-discretized path probability for the Euler-Maruyama integrator

$$P[\mathbf{x},\alpha] = p(x_0,\alpha)\cdot \mathcal{P}[x_1 \dots x_n|\, x_0,\alpha] = p(x_0,\alpha)\cdot \prod_{k=1}^{n-1} p(x_{k+1}|x_k,\alpha)$$

$$p(x_0,\alpha) = \frac{1}{Z(\alpha)}\exp(-\beta V(x,\alpha))$$

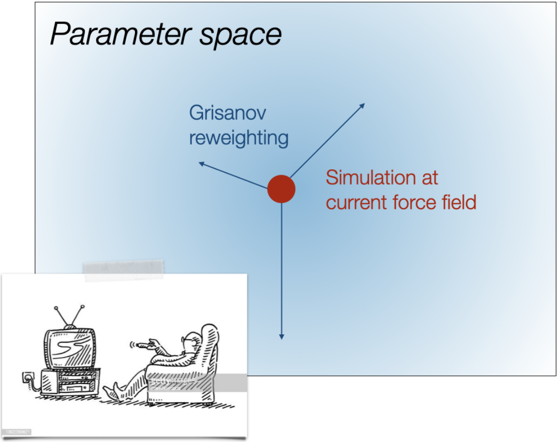
$$p(x_{k+1}|x_k,\alpha) = \sqrt{\frac{\xi m}{4\pi k_B T\Delta t}}\cdot \exp\left(-\frac{\xi m}{4k_B T\Delta t}\left(x_{k+1}-x_k+\frac{\Delta t}{\xi m}\frac{d}{dx}V(x_k,\alpha)\right)^2\right)$$

Path reweighting factor

$$\frac{Z}{Z(\alpha)}W[\mathbf{x},\alpha] = \frac{p(x_0,\alpha)}{p(x_0,,\alpha=0)}\prod_{k=0}^{n-1}\frac{p(x_{k+1}|\, x_k,\alpha)}{p(x_{k+1}|\, x_k,\alpha=0)}$$

L. Onsager, S. Machlup (1953), V. Girsanov (1960), D. M. Zuckerman, T. B. Woolf (1999, 2000), C. Xing, I. Andricioaei (2006), B. Adib (2008), Schütte (2015)
L. Donati, C. Hartmann, **BGK**, *J. Chem. Phys.* **2017**, *146*, 244112, L. Donati, **BGK**, *J Chem Phys*, **2018**, *149*, 072335
S. Kieninger, **BGK** *J. Chem. Phys*, **2021**, *154*, 094102. S. Kieninger, L. Donati, **BGK**, *Curr. Opin. Struct. Biol.*, **2020**, *61*, 124-131

“Zapping” through parameter space is inefficient for molecular force fields



General idea:
Take a simulation at the current FF and use Girsanov reweighting to calculate the kinetic properties at different FF parameter values.

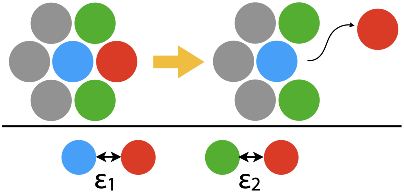
But the parameter space is high-dimensional!

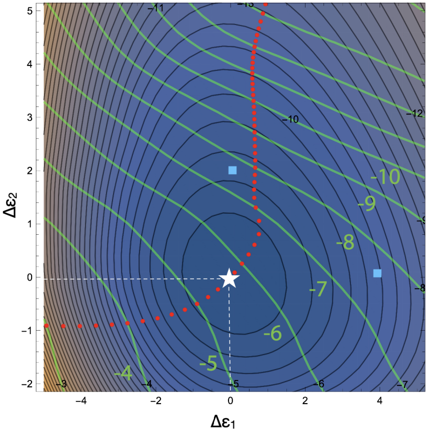
- We need a property that guides the search through parameter space.
- Several parameter combination will yield the same rate. We need a criterion to choose among them.

Maximum caliber / maximum path entropy
&
path reweighting

P.G. Bolhuis, Z.F. Brotzakis, Bettina G. Keller,
Force field optimization by imposing kinetic constraints with path reweighting
arXiv preprint **2022**, arXiv:2207.04558.

2D dissociation model





- white star: current force field
- color gradient: distance to the current force field
- green lines: parameters that yield the same unbinding rate k_{AB}
- red dots: parameter combinations with minimal distance to the current force field that fullfill a constraint for k_{AB}.

Goal: Solve this optimization problem without re-simulating the system.

$$k_{AB} = \frac{\phi_A \int_A \mathcal{D}\mathbf{x}\, P[\mathbf{x}]\theta(\lambda_{\max - \lambda_B}[\mathbf{x}])}{\int_A \mathcal{D}\mathbf{x}\, P[\mathbf{x}]}$$

Maximum caliber approach

Kullback-Leibler divergence D_{KL} or relative path entropy S

$$D_{KL}(\mathbf{a}) = -S[P[\mathbf{x},\mathbf{a}]|\; P[\mathbf{x}]] = \int \mathcal{D}\mathbf{x}\, P[\mathbf{x},\mathbf{a}] \ln \frac{P[\mathbf{x},\mathbf{a}]}{P[\mathbf{x}]}$$

measure the deviation of the path probability $P[\mathbf{x},\mathbf{a}]$ from the path probability of the current force field $P[\mathbf{x}]$.

→ find the extremum of D_{KL} or S under the constraints that

- $\langle s \rangle$ fulfills an experimental constraint s_{exp}
- $P[\mathbf{x},\mathbf{a}]$ remains normalized.

Path Lagrange function

$$\mathcal{L}(\mathbf{a}) = D_{KL}(\mathbf{a}) - \mu \left(\int \mathcal{D}\mathbf{x}\, P[\mathbf{x},\mathbf{a}] s(\mathbf{x}) - s_{\mathrm{exp}} \right) - \nu \left(\int \mathcal{D}\mathbf{x}\, P[\mathbf{x},\mathbf{a}] - 1 \right)$$

solve

$$\frac{\partial}{\partial a_k} D_{KL}(\mathbf{a}) = 0, \quad \frac{\partial}{\partial \mu} D_{KL}(\mathbf{a}) = 0, \quad \frac{\partial}{\partial \nu} D_{KL}(\mathbf{a}) = 0$$

E.T. Jaynes (1980), , G. Stock (2010), K. Dill, PD. Dixit, S. Pressé, K. Gosh *et. al.* (2013, 2015 , 2018), P. G. Bolhuis, Z. Faidon Brotzakis , M. Vendruscolo (2020, 2021)
P.G. Bolhuis, Z.F. Brotzakis, **BGK**, *arXiv preprint* **2022**, arXiv:2207.04558.

Reweighting the path Lagrange function $\mathcal{L}(\mathbf{a})$

1. Choose $P[\mathbf{x},\mathbf{a}]$ to be normalized

$$P[\mathbf{x},\mathbf{a}] = \frac{Z}{Z(\mathbf{a})} W[\mathbf{x},\mathbf{a}] P[\mathbf{x}]$$

2. Reweight the path expected value

$$\langle s\rangle_{\mathbf{a}} = \int \mathcal{D}\mathbf{x}\, P[\mathbf{x},\mathbf{a}] s(\mathbf{x}) = \int \mathcal{D}\mathbf{x}\, \frac{Z}{Z(\mathbf{a})} W[\mathbf{x},\mathbf{a}] P[\mathbf{x}] s(\mathbf{x})$$

3. Reweight the Kullback-Leibler divergence

$$D_{KL}(\mathbf{a}) = \frac{\mathcal{Z}}{\mathcal{Z}(\mathbf{a})} \int \mathcal{D}\mathbf{x}\, W[\mathbf{x};\mathbf{a}]\mathcal{P}[\mathbf{x}] \,\ln\left[\frac{\mathcal{Z}}{\mathcal{Z}(\mathbf{a})} W[\mathbf{x};\mathbf{a}] \frac{\mathcal{P}[\mathbf{x}]}{\mathcal{P}[\mathbf{x}]}\right] = \langle \ln W[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}} - \ln \frac{\mathcal{Z}(\mathbf{a})}{\mathcal{Z}}$$

Then

$$\mathcal{L}(\mathbf{a}) = \langle \ln W[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}} - \ln \frac{\mathcal{Z}(\mathbf{a})}{\mathcal{Z}} - \mu(\langle s\rangle_{\mathbf{a}} - s_{\mathrm{exp}})$$

Slightly adjust the constraint to the experimental value

$$\mathcal{L}(\mathbf{a}) = \langle \ln W[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}} - \ln \frac{\mathcal{Z}(\mathbf{a})}{\mathcal{Z}} - \mu(\ln\langle s\rangle_{\mathbf{a}} - \ln s_{\mathrm{exp}})$$

P.G. Bolhuis, Z.F. Brotzakis, **BGK**, *arXiv preprint* **2022**, arXiv:2207.04558.

Term 1: $\ln W[\mathbf{x};\mathbf{a}]$ is a path observable $w[\mathbf{x},\mathbf{a}]$

Path reweighting factor

$$\frac{Z}{Z(\mathbf{a})} W[\mathbf{x},\mathbf{a}] \quad = \quad \frac{p(x_0,\mathbf{a})}{p(x_0,,\mathbf{a}=0)} \prod_{k=0}^{n-1} \frac{p(x_{k+1}|\, x_k,\mathbf{a})}{p(x_{k+1}|\, x_k,\mathbf{a}=0)}$$

Euler-Maruyama in 1D, analogous for nD, potential $V(x)+U(x,\mathbf{a})$

$$\frac{p(x_0,\mathbf{a})}{p(x_0,,\mathbf{a}=0)} \quad = \quad \frac{Z}{Z(\mathbf{a})} \exp\left(-\frac{1}{k_B T} U(x,\mathbf{a})\right)$$

$$\frac{p(x_{k+1}|\, x_k,\mathbf{a})}{p(x_{k+1}|\, x_k,\mathbf{a}=0)} \quad = \quad \exp\left(-\kappa \eta_k \nabla U(x_k,\mathbf{a})\right) \exp\left(-\frac{1}{2}\kappa^2 \left(\nabla U(x_k,\mathbf{a})\right)^2\right)$$

with

- η_k is the random number of the integration step
- $\kappa = \sqrt{2/k_B T \xi m}$, where ξ is a collision frequency with unit s^{-1}, Δt is the integration time step.

L. Donati, C. Hartmann, **BGK**, *J. Chem. Phys.* **2017**, *146*, 244112, L. Donati, **BGK**, *J Chem Phys*, **2018**, *149*, 072335
S. Kieninger, **BGK** *J. Chem. Phys*, **2021**, *154*, 094102. S. Kieninger, L. Donati, **BGK**, *Curr. Opin. Struct. Biol.*, **2020**, *61*, 124-131
P.G. Bolhuis, Z.F. Brotzakis, **BGK**, *arXiv preprint* **2022**, arXiv:2207.04558.

Term 1: $\ln W[\mathbf{x};\mathbf{a}]$ is a path observable $w[\mathbf{x},\mathbf{a}]$

$\ln W[\mathbf{x};\mathbf{a}]$ simplifies

$$W[\mathbf{x};\mathbf{a}] = \exp\left(-\frac{1}{k_BT}U(x,\mathbf{a})\right)\exp\left(-\sum_{k=0}^{n-1}\kappa\eta_k\nabla U(x_k,\mathbf{a})\right)\exp\left(-\frac{1}{2}\sum_{k=0}^{n-1}\kappa^2\left(\nabla U(x_k,\mathbf{a})\right)^2\right)$$

$$w[\mathbf{x};\mathbf{a}] = \ln W[\mathbf{x};\mathbf{a}] = -\frac{1}{k_BT}U(x_0,\mathbf{a}) - \sum_{k=0}^{n-1}\kappa\eta_k\nabla U(x_k,\mathbf{a}) - \frac{1}{2}\sum_{k=0}^{n-1}\kappa^2\left(\nabla U(x_k,\mathbf{a})\right)^2$$

and

$$w'[\mathbf{x};\mathbf{a}] = \frac{\partial}{\partial a_k}w[\mathbf{x};\mathbf{a}] = -\frac{1}{k_BT}\frac{\partial}{\partial a_k}U(x_0,\mathbf{a}) - \sum_{k=0}^{n-1}\kappa\eta_k\frac{\partial}{\partial a_k}\nabla U(x_k,\mathbf{a}) - \sum_{k=0}^{n-1}\kappa^2\frac{\partial}{\partial a_k}\left(\nabla U(x_k,\mathbf{a})\cdot\frac{\partial}{\partial a_k}\nabla U(x_k,\mathbf{a})\right)$$

... after some algebra

$$\frac{\partial}{\partial a_k}\langle\ln W[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}} = -\langle w'[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}}\langle w[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}} + \langle w'[\mathbf{x};\mathbf{a}]w[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}} + \langle w'[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}}$$

P.G. Bolhuis, Z.F. Brotzakis, **BGK**, *arXiv preprint* **2022**, arXiv:2207.04558.

The derivatives of the path Lagrange function $\mathcal{L}(\mathbf{a})$

Path Lagrange function

$$\mathcal{L}(\mathbf{a}) = \langle \ln W[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}} - \ln \frac{\mathcal{Z}(\mathbf{a})}{\mathcal{Z}} - \mu(\ln\langle s\rangle_{\mathbf{a}} - \ln s_{\mathrm{exp}})$$

Derivatives of the individual terms

$$\begin{aligned}
\frac{\partial}{\partial a_k}\langle \ln W[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}} &= -\langle w'[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}}\langle w[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}} + \langle w'[\mathbf{x};\mathbf{a}]w[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}} + \langle w'[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}} \\
-\frac{\partial}{\partial a_k}\ln\frac{\mathcal{Z}(\mathbf{a})}{\mathcal{Z}} &= -\langle w'[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}} \\
-\frac{\partial}{\partial a_k}\mu\ln\langle s\rangle_{\mathbf{a}} &= -\mu\left[-\langle w'[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}} + \langle w'[\mathbf{x};\mathbf{a}]\rangle_{s\mathbf{a}}\right] \\
-\frac{\partial}{\partial a_k}\ln s_{\mathrm{exp}} &= 0
\end{aligned}$$

$$\langle w'[\mathbf{x};\mathbf{a}]\rangle_{s\mathbf{a}} = \frac{\int \mathcal{D}\mathbf{x} P W w' s}{\int \mathcal{D}\mathbf{x} P W s}$$

Derivatives of the path Lagrange function as reweighted path integrals

$$\begin{aligned}
\frac{\partial}{\partial a_k}\mathcal{L}(\mathbf{a}) &= -\langle w'[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}}\langle w[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}} + \langle w'[\mathbf{x};\mathbf{a}]w[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}} - \mu\left[\langle w'[\mathbf{x};\mathbf{a}]\rangle_{s\mathbf{a}} - \langle w'[\mathbf{x};\mathbf{a}]\rangle_{\mathbf{a}}\right] \\
\frac{\partial}{\partial \mu}\mathcal{L}(\mathbf{a}) &= \ln\langle s\rangle_{\mathbf{a}} - \ln s_{\mathrm{exp}}
\end{aligned}$$

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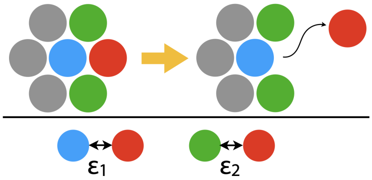
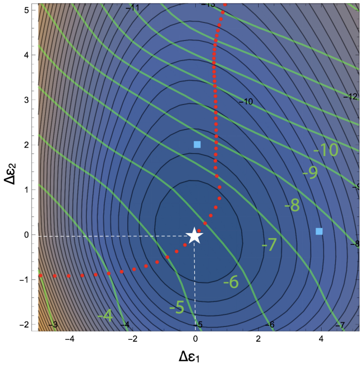
2D dissociation model - tuning the force field

Reference force field

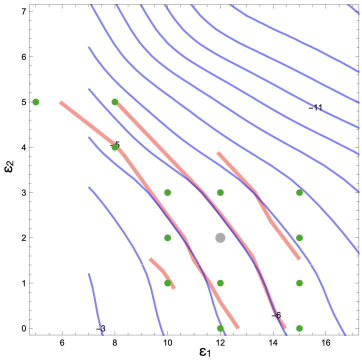


- gray particles flexible
- ○ ↔ ○ : $\epsilon_1 = 12\,k_B T, \sigma = 1.0\,\mathrm{unitlength}$
- ○ ↔ ○ : $\epsilon_2 = 2\,k_B T, \sigma = 1.0\,\mathrm{unitlength}$

MaxCal & Reweighting



Sampling



green dots: direct simulations
red lines: interpolated iso-rate lines
blue lines: iso-rate lines from MaxCal & path reweighting

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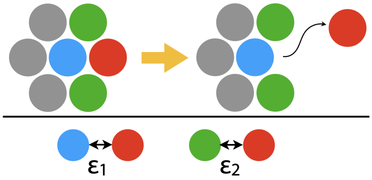
Learning about the dynamics

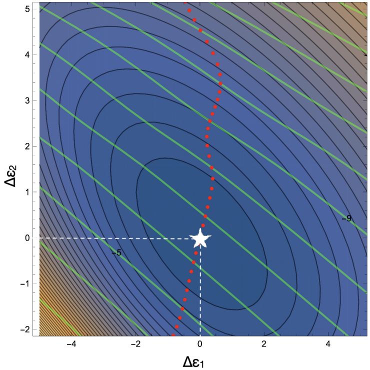
2D dissociation model: fixed gray particles

Reference force field



- gray particles fixed
- ○ ↔ ○ : $\epsilon_1 = 10\, k_B T, \sigma = 1.0\,\mathrm{unitlength}$
- ○ ↔ ○ : $\epsilon_2 = 1\, k_B T, \sigma = 1.0\,\mathrm{unitlength}$

MaxCal & Reweighting

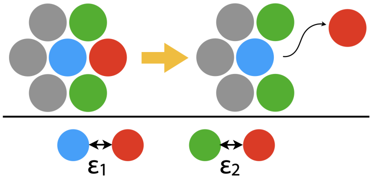


- iso-rate lines roughly linear with slope ~ 0.5.
- $\Delta\epsilon_1 = 2\, k_B T$ requires $\Delta\epsilon_2 = 1\, k_B T$: one blue, two green particles
- line of optimal parameters almost vertical → indepedent of increasing or decreasing the rate, changing ϵ_2 perturbs the path ensemble the least
- all transition paths are affected by ϵ_1, but only successful transition paths are affected by ϵ_2

P.G. Bolhuis, Z.F. Brotzakis, **BGK**, *arXiv preprint* **2022**, arXiv:2207.04558.

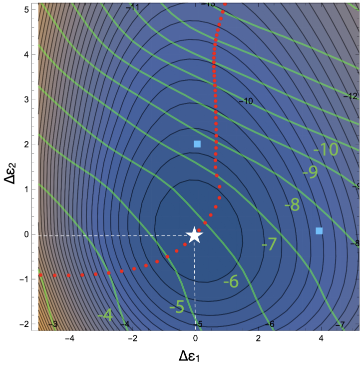
2D dissociation model: flexible gray particles

Reference force field



- gray particles flexible
- $\circ \leftrightarrow \circ$: $\epsilon_1 = 12\, k_B T, \sigma =$ 1.0 unit length
- $\circ \leftrightarrow \circ$: $\epsilon_2 = 2\, k_B T, \sigma =$ 1.0 unit length

MaxCal & Reweighting

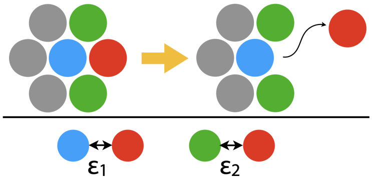


- iso-rate lines follow the same trend as before, but less linear
- line of optimal parameters roughly diagonal for $\Delta\epsilon_{1,2} = \pm 1\, k_B T \rightarrow$ both parameters contribute to tuning the rate.
- increasing the rate further: only ϵ_1 contributes, ϵ_1 is scaled down
- decreasing the rate further: only ϵ_2 contributes, ϵ_2 is scaled up
- For decreasing the rate changing the association to the green particles is sufficient, and has only mild effect on the path ensemble.
- For increasing the rate, setting ϵ_2 to zero, will not be sufficient. ϵ_1 needs to be altered as well.

P.G. Bolhuis, Z.F. Brotzakis, **BGK**, *arXiv preprint* **2022**, arXiv:2207.04558.

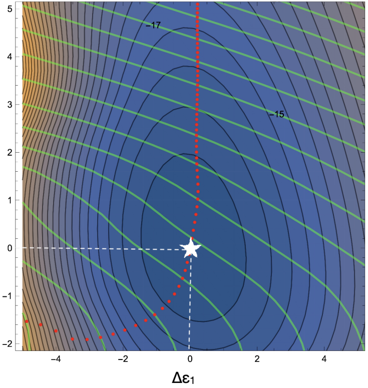
2D dissociation model: flexible gray particles, reference force field binds more strongly

Reference force field



- gray particles flexible
- $\circ \leftrightarrow \circ$: $\epsilon_1 = 15\,k_B T, \sigma =$ 1.0 unit length
- $\circ \leftrightarrow \circ$: $\epsilon_2 = 5\,k_B T, \sigma =$ 1.0 unit length

MaxCal & Reweighting

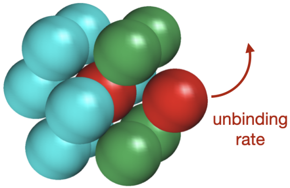


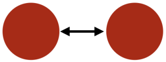
- similar trends as before

P.G. Bolhuis, Z.F. Brotzakis, **BGK**, *arXiv preprint* **2022**, arXiv:2207.04558.

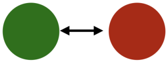
3D Lennard-Jones cluster

Dissociation in a 3D Lennard-Jones cluster





ϵ_1



ϵ_2

Fixed blue particles

- blue particles flexible
- $\epsilon_1 = 12\, k_B T, \sigma = 1.0\,\text{unit length}$
- $\epsilon_2 = 1\, k_B T, \sigma = 1.0\,\text{unit length}$

Flexible blue particles, shallow binding minimum

- blue particles flexible
- $\epsilon_1 = 12\, k_B T, \sigma = 1.0\,\text{unit length}$
- $\epsilon_2 = 2\, k_B T, \sigma = 1.0\,\text{unit length}$

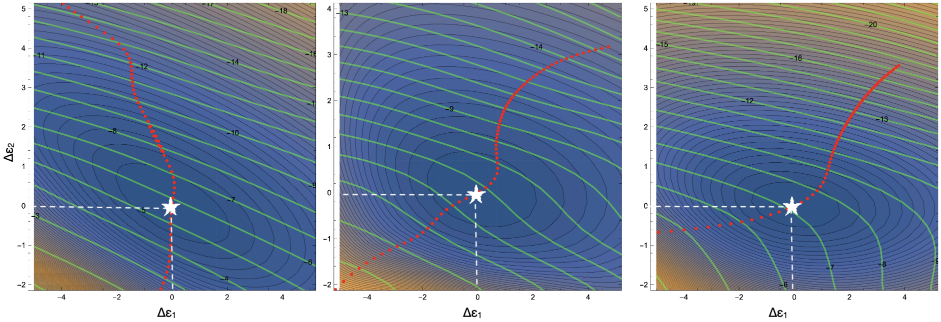
Flexible blue particles, shallow binding minimum

- blue particles flexible
- $\epsilon_1 = 12\, k_B T, \sigma = 1.0\,\text{unit length}$
- $\epsilon_2 = 2\, k_B T, \sigma = 1.0\,\text{unit length}$

P.G. Bolhuis, Z.F. Brotzakis, **BGK**, *arXiv preprint* **2022**, arXiv:2207.04558.

Dissociation in a 3D Lennard-Jones cluster

Fixed blue particles | Flexible blue particles shallow minimum | Flexible blue particles deep minimum



Similar effects and trends as in the 2D model.
Outer particles are prime targets for reducing the rate.

P.G. Bolhuis, Z.F. Brotzakis, **BGK**, *arXiv preprint* **2022**, arXiv:2207.04558.

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Post-Doc position available!

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