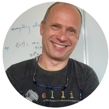
From biased to unbiased dynamics: slow dynamical modes from static averages

September 16, 2025

Timothée Devergne

Vladimir Kostic


Massimiliano Pontil

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Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA

FAIR Future Artificial Intelligence Research

Outline

1 Overview: what is our aim here?

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5. Blind discovery of metastable states

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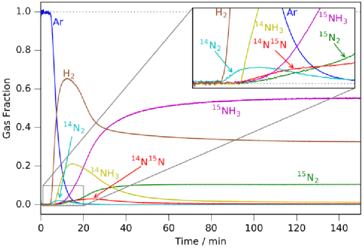

Wood *et al.*, **Phys. Chem. Chem. Phys.**, 2017, 19, 4719-4724

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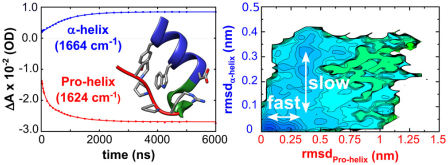

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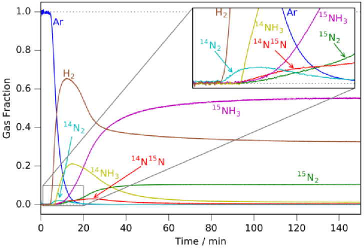

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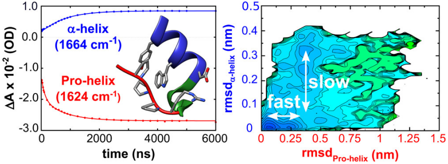

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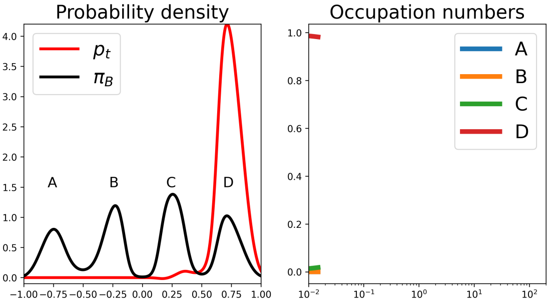
A probabilistic view on using data from molecular dynamics to study time evolution of systems

Occupation numbers are related to probability distributions

Occupation number of state A at time t $\mathbb{1}_A(t)$: $\mathbb{1}_{\mathbb{A}}(t) = \int_{x \in A} p_t(x)dx$

p_t: Probability distribution at time t, converges towards the Boltzmann one for $t \to \infty$


Probability density
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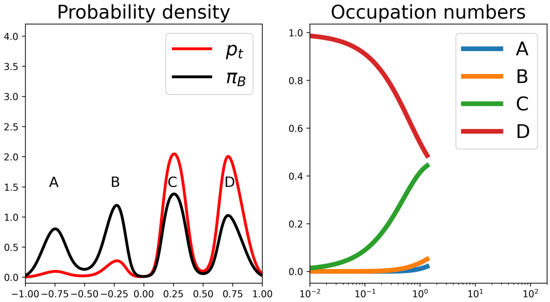
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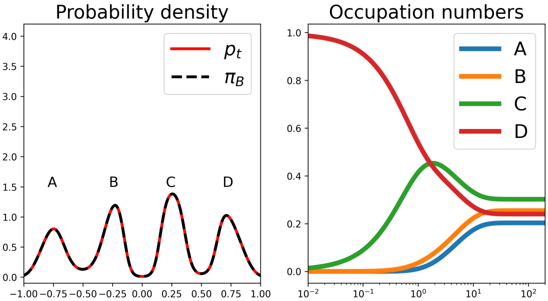

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Occupation numbers

- Knowing p_t gives access to the time evolution of any observable
- Starting in a given state, how will the occupation number evolve with time?
- This is for a very simple system, how can we have p_t for multidimensional systems

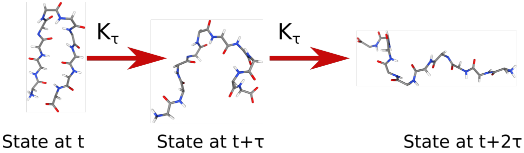
The Koopman/Transfer Operator from Unbiased Simulations

Given a Markov process, define

$$u_t = \frac{p_t}{\pi},$$

then the Koopman operator K_τ propagates u_t forward in time:

$$u_{t+\tau} = K_\tau u_t \quad \Longrightarrow \quad u_{n\tau} = (K_\tau)^n u_0.$$



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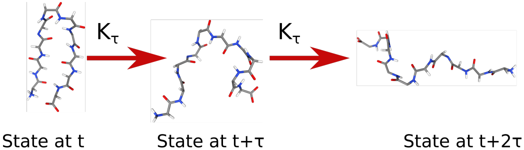


Learning K_τ: Several approaches exist (EDMD, kernel methods, VAMP, etc.):

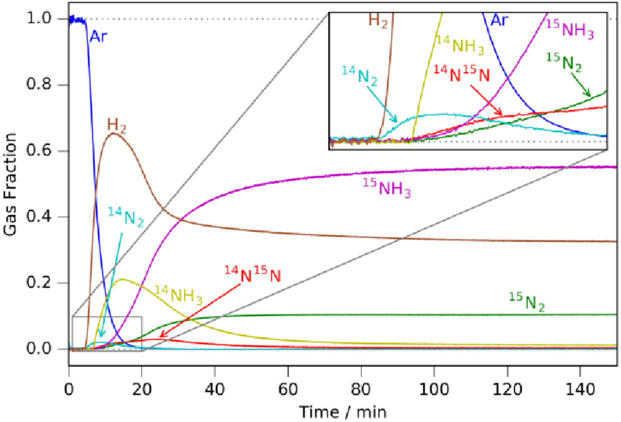
- Schütte et al., Springer, 1999
- Mardt *et al.*, Nature Communications, 2018
- Kostic *et al.*, ICLR 2024

All require: The evaluation of the time-lagged correlation function

$$C(\tau) = \int \psi(x_t)\,\psi(x_{t+\tau})\,dt,$$

where ψ is a chosen observable.

Time evolution of reactions



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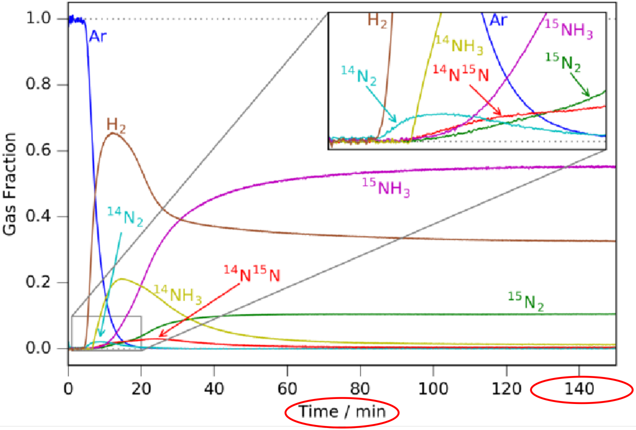

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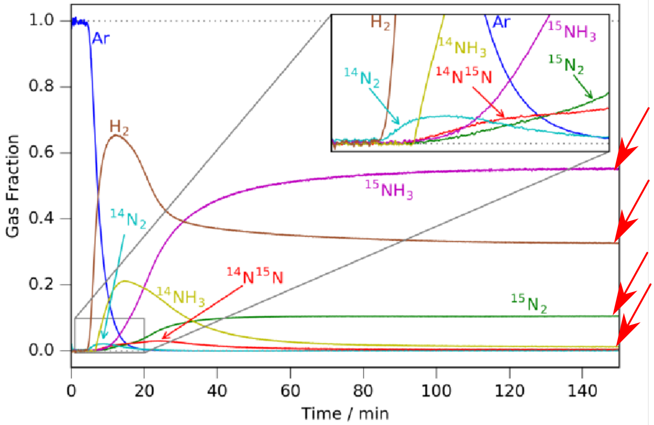
- Transition mechanisms often involve several steps
- They are rare events
- The typical timestep of a simulation : $0.2 \rightarrow 2fs$
- 100 minutes would mean $\approx 6.10^{18}$ timesteps which is not possible
- Some form of enhanced sampling scheme is needed

What observable can we get from a single long biased simulations



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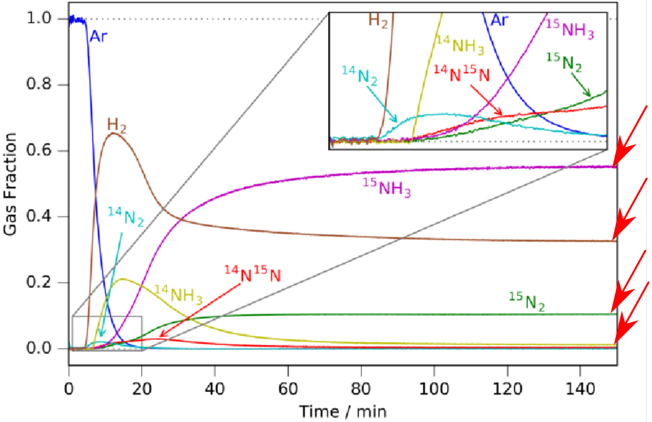

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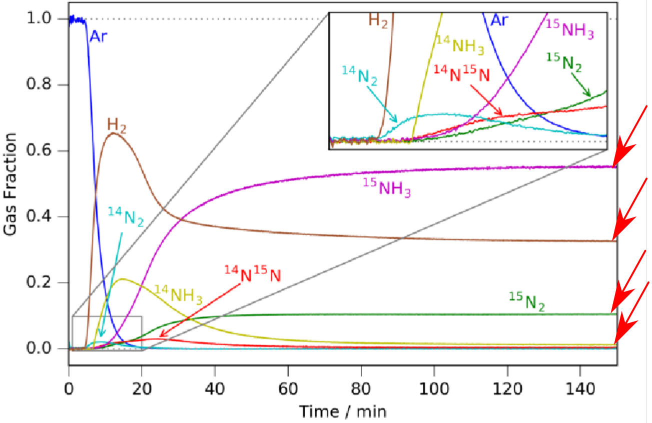

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- The free energy profile gives occupation numbers at equilibrium
- An estimate of the rates can be obtained by the free energy barrier
- How can we get the time evolution of the occupation numbers of the states?
- $C_{biased}(\tau) \neq C_{unbiased}(\tau)$

Is there a differential equation for u_t?

From discrete to continuous time

$$u_{t+\tau} = K_\tau \, u_t$$

The difficulty: we need u at both t and $t+\tau$. What happens as $\tau \to 0 : \frac{\partial u_t}{\partial t}$?

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Langevin dynamics assumption

There is a closed-form equation: $\frac{\partial u_t}{\partial t} = \mathcal{L} u_t$

$\mathcal{L}$ is the **infinitesimal generator** of the dynamics (backward Kolmogorov equation):

$$\mathcal{L} f(\mathrm{R}) = \frac{1}{\gamma} \sum_{i=1}^{N} \frac{1}{m_i} \frac{\partial f(\mathrm{R})}{\partial r_i} \frac{\partial U(\mathrm{R})}{\partial r_i} - \frac{1}{\beta\gamma} \sum_{i=1}^{N} \frac{1}{m_i} \frac{\partial^2 f(\mathrm{R})}{\partial r_i^2}$$

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- $\mathcal{L}$ depends linearly on the potential U
- But this formulation is cumbersome and only tractable in low dimensions

Modal decomposition of $\mathcal{L}$

$\mathcal{L}$ can be decomposed into eigenvectors and eigenvalues which give insights about the dynamical behavior:

$$\mathcal{L}\psi_i(\mathrm{R}) = \lambda_i\psi_i(\mathrm{R}), \quad 0 = \lambda_0 < \lambda_1 < \lambda_2 < \dots$$

$$u_t(\mathrm{R}) = \sum_i \psi_i(\mathrm{R})e^{-\lambda_i t} \langle\psi_i|u_0\rangle$$

$\langle\psi_i|u_0\rangle = \int \psi_i(\mathrm{R})u_0(\mathrm{R})\frac{e^{-\beta U(\mathrm{R})}}{Z}d\mathrm{R}$

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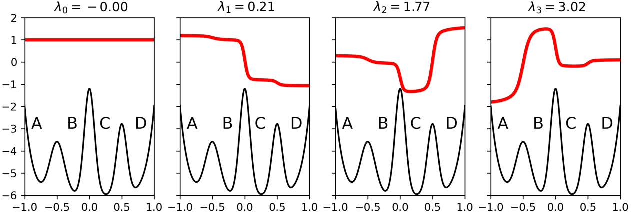

The problem is transformed from a PDE to an eigenvalue problem

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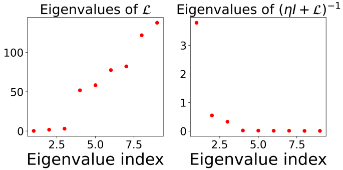

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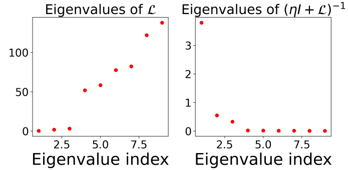

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$\mathcal{L}$ involves second derivatives

We will use the Dirichlet form:

$$\langle\psi|\mathcal{L}|\phi\rangle = -\frac{1}{\beta\gamma}\int \nabla_{\mathbf{u}}\phi(\mathbf{R})\nabla_{\mathbf{u}}\psi(\mathbf{R})\frac{e^{-\beta U(\mathbf{R})}}{Z}d\mathbf{R}$$

Dirichlet

Kolmogorov

Operator learning

Given a set of functions $|\phi_i\rangle$, one will try to find the matrix G such that

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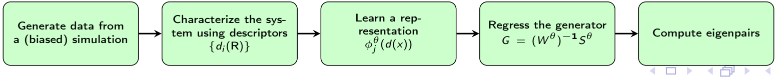
The $|\phi_i\rangle$ are learned by using neural networks, minimizing the loss $Tr(S^\theta\Lambda^\theta W^\theta\Lambda^\theta - 2S^\theta\Lambda^\theta) + Tr((S^\theta - I)^2)$

Boltzmann distribution is all we need

There is no time dependance, it is replaced with the differential operator, only Boltzmann averages are needed.



Generate data from a (biased) simulation

Characterize the system using descriptors $\{d_i(\mathrm{R})\}$

Learn a representation $\phi_j^\theta(d(x))$

Regress the generator $G = (W^\theta)^{-\mathbf{1}}S^\theta$

Compute eigenpairs

Alanine dipeptide: first eigenfunction as CV

Test of this method on a model system: alanine dipeptide

- ϕ is known to be good collective variable: biasing with it will lead to many transitions
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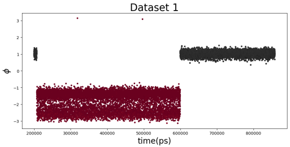

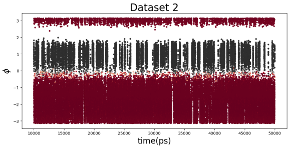

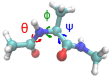

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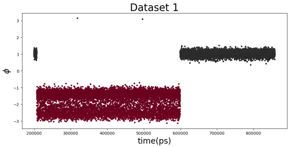
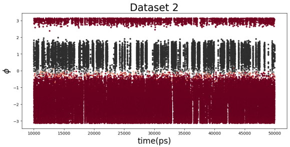
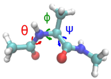
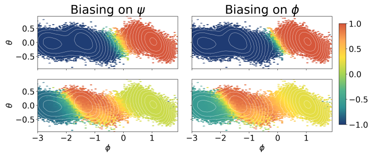








Conclusion

We can obtain a good estimate of where the transition region is, even with a sparse dataset

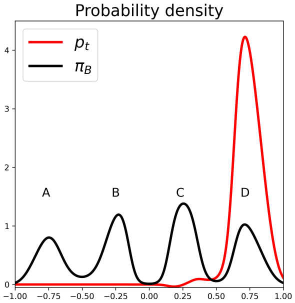
Time evolution of observables

We start from a system in a metastable state A and we want to know its relaxation towards the Boltzmann distribution:

The initial distribution is the Boltzmann one restricted to state D:

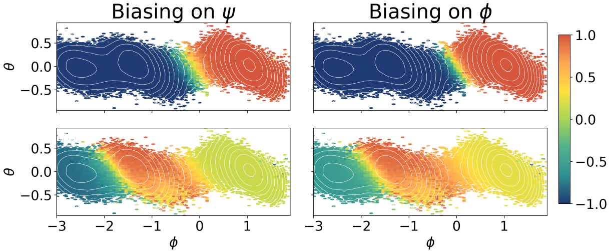
$$p_0^D(\mathrm{R}) = \frac{e^{-\beta U(\mathrm{R})}}{\int_{\mathrm{R}\in D} e^{-\beta U(\mathrm{R})}} \mathbb{1}_D(\mathrm{R}) \text{ hence } u_0^D(\mathrm{R}) = \frac{Z}{Z_A} \mathbb{1}_D(\mathrm{R})$$

$$\mathrm{u}_t(\mathrm{R}) = \sum_{i=0}^m \psi_i(\mathrm{R}) e^{-\lambda_i t} \langle \psi_i | u_0 \rangle$$



Time evolution of alanine dipeptide

The sign of eigenfunctions can be used to classify states due to the relation of $\int \psi_i(\mathrm{R}) \frac{e^{-\beta U(\mathrm{R})}}{Z} d\mathrm{R} = 0$



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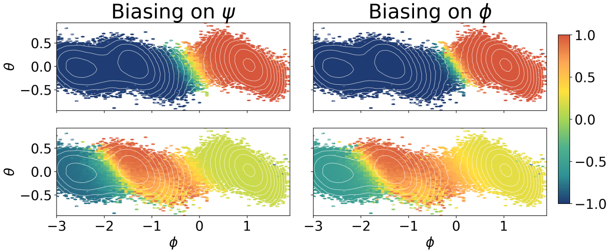
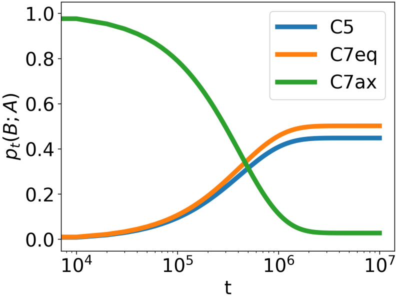


And forecast time evolution of occupation numbers



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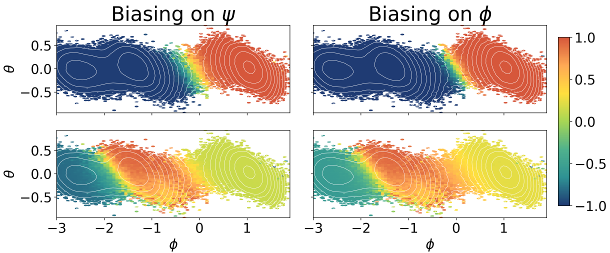

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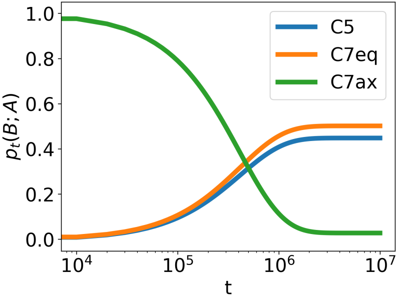
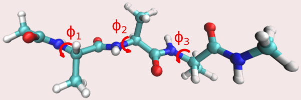


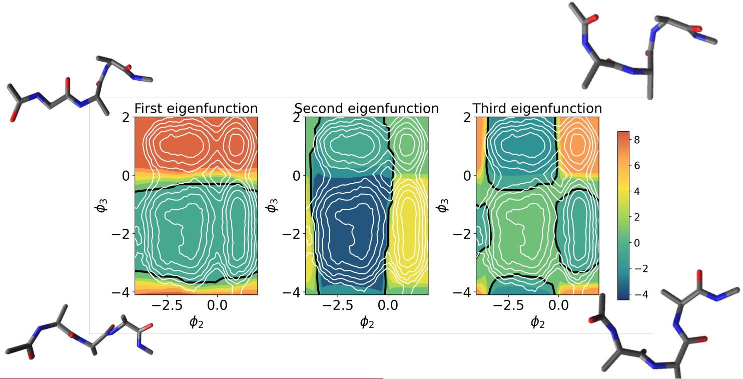
From an initial propability distribution in the least occupied state, we can forecast how the other state will evolve. Can we do it for systems with a higher number of states?

Alanine tetrapeptide

Alanine tetrapeptide is a simple molecule displaying several states



Identification of the states



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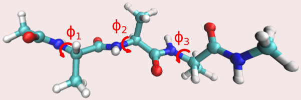

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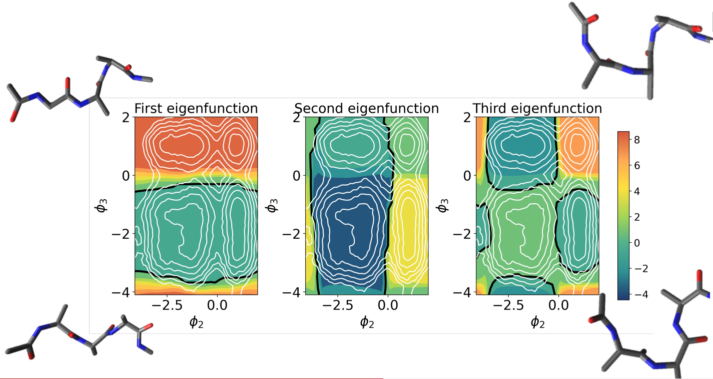
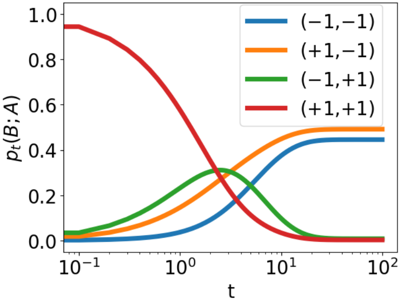


Forecasting occupation numbers

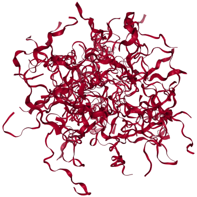


Until there: only small molecules for which we already know the results.

Application: Intrinsically disordered proteins.

IDPs are proteins that do not have a fixed stable 3D structure.

- Disorder is present in 70% of proteins
- They are involved in many cancers and degenerative diseases like Alzheimer or Parkinson
- Considered undrugable due to the high number of conformations they can adopt
- ML models (alphafold..) describe them poorly



Peptone

M. Invernizzi and S. Bottaro

Application: IDPs Aβ42

Aβ42 is a 42 residues IDP involved in Alzheimer disease: finding its most stable states is key. For this study, we used a publicly available (unbiased) trajectory Lohr *et al* Nature Computational Science (2021).

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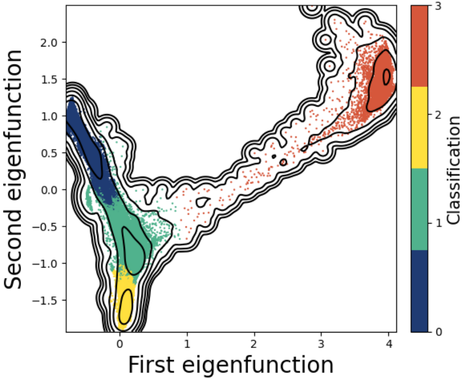
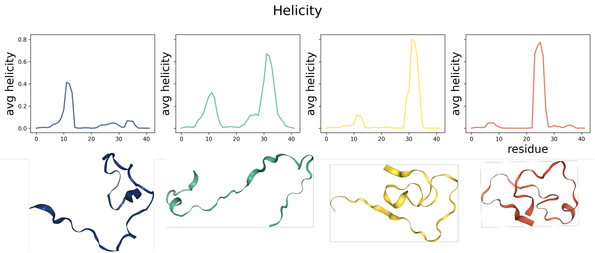
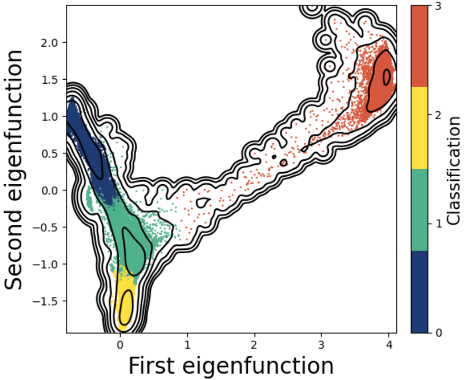


Are these states physically meaningful ? Let us look at the secondary structures

Application: IDPs Aβ42 secondary structure

All states are related to a secondary structure change.





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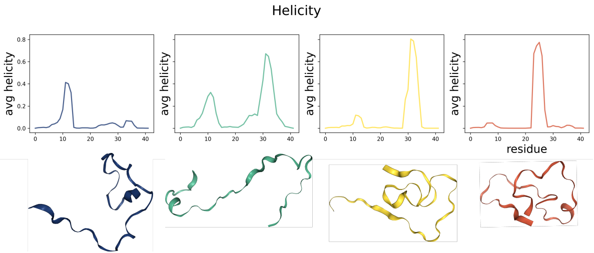

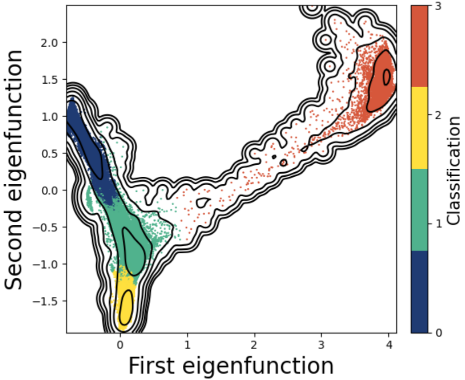

We can associate each mode with a structural change, **because the eigenfunctions contain the relevant long time dynamical behavior information**

Conclusion I

Main idea

- Compute dynamical properties directly from Boltzmann-distributed samples
- In principle, applicable with *any* data generation scheme

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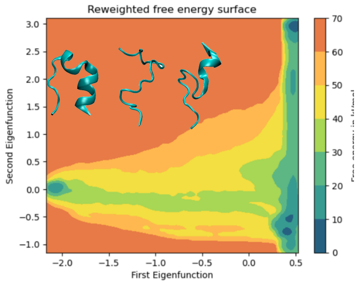

Can we start from only one state?

The loss

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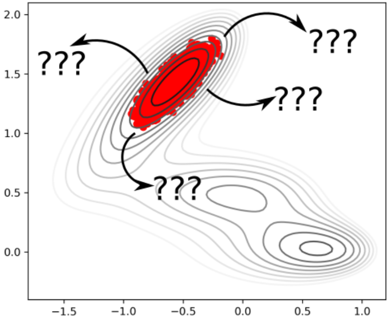
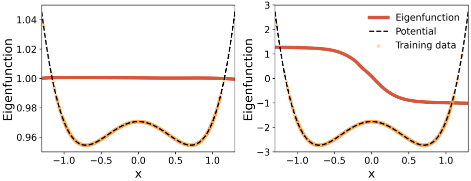
Is this only a postprocessing tool?



Our initial observation

At high temperature, when the whole landscape is sampled:



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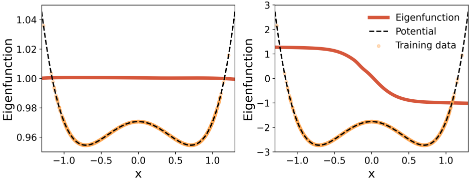

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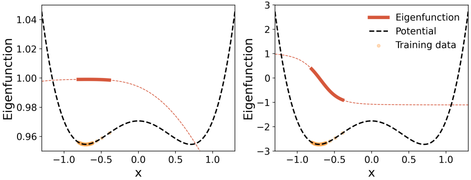

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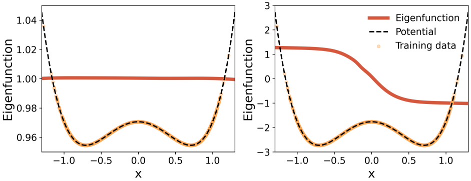

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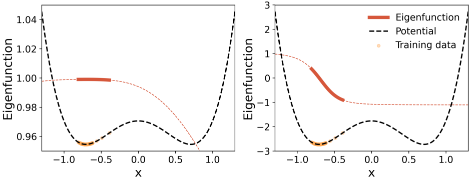

We use what is thought to be a pain for neural networks: their poor extrapolation capabilities

Use the curvature that defines the unexplored space:

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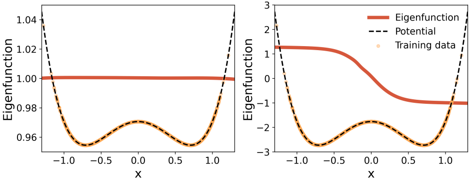

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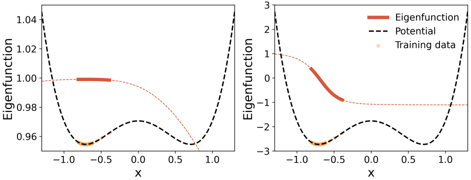

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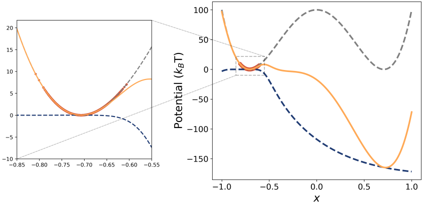
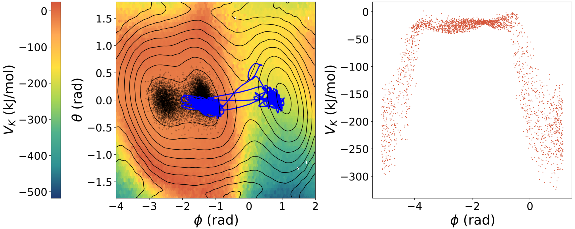


$V_K(x)$ is called the Kolmogorov bias (Kang *et al*, Nature Computational Science, 2024).

Proof of concept: alanine dipeptide

We mix V_K with an OPES bias to push the system out of the initial basin



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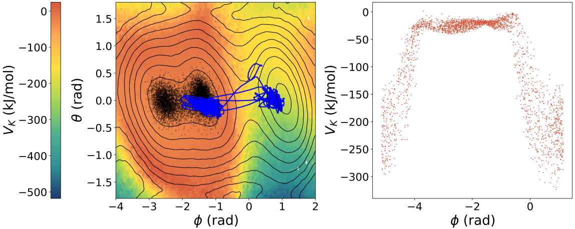

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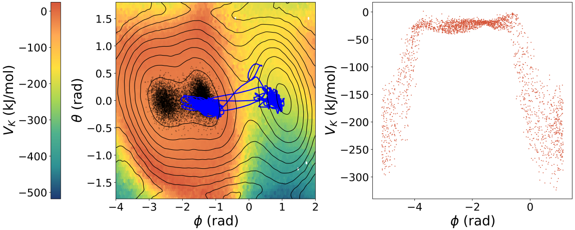

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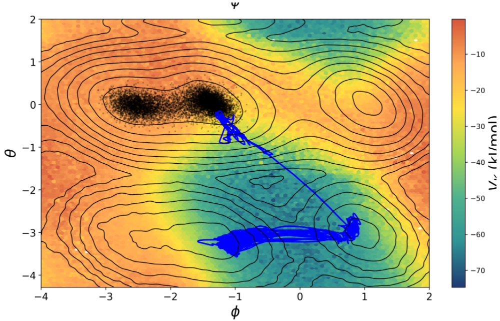

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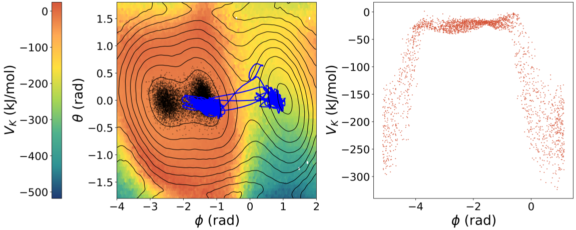

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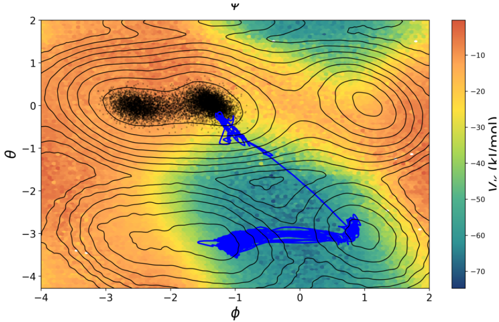
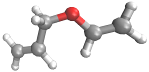


Discovering chemical reactions

Given an initial reactant, how to predict the possible products 

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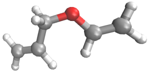

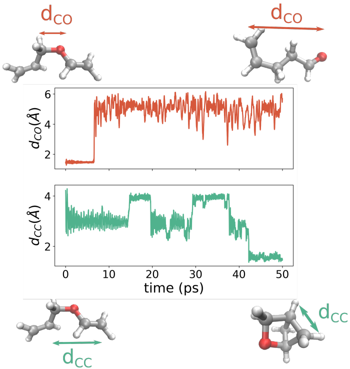

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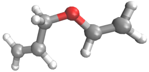

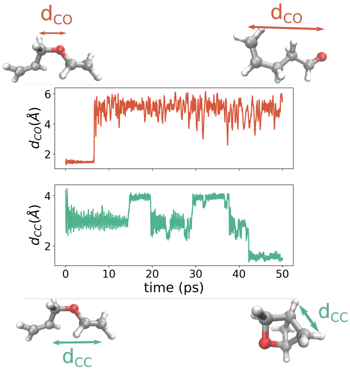

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Possible application

Prebiotic chemistry: how did bioprecursors form on earth

Conclusions

Take-home messages

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mlcolvar

Implementation in mlcolvar
Thanks to Enrico Trizio

Code snippet

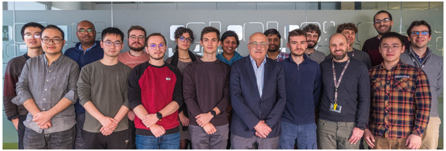
```
smart_derivatives = SmartDerivatives(force_all_atoms=True)
smart_dataset = smart_derivatives.setup(
    dataset, ComputeDistances, n_atoms,
    descriptors_batch_size=1000, positions_noise=1e-4)

model = Generator(
    layers=[45,20,20,1], eta=0.005, r=3, alpha=0.005,
    friction=friction, descriptors_derivatives=smart_derivatives,
    options=options, u_stat=True, cell=cell)
```

Joyeux anniversaire Michele

"Grazie per la tua pazienza"

Thank you



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