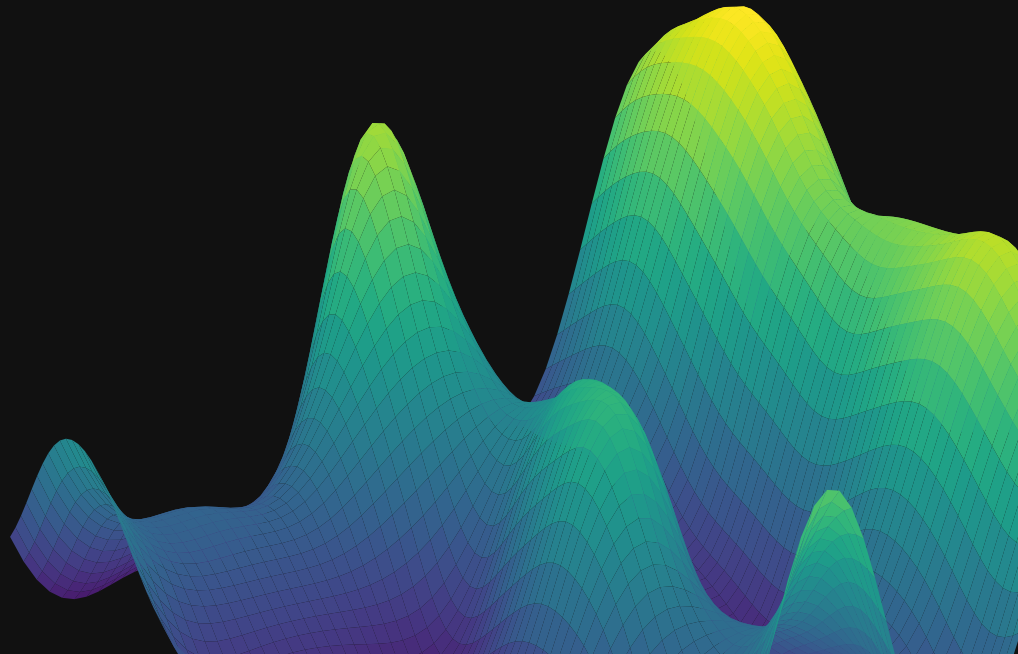
PySAGES
Enhanced Sampling Molecular Dynamics Simulations on GPUs

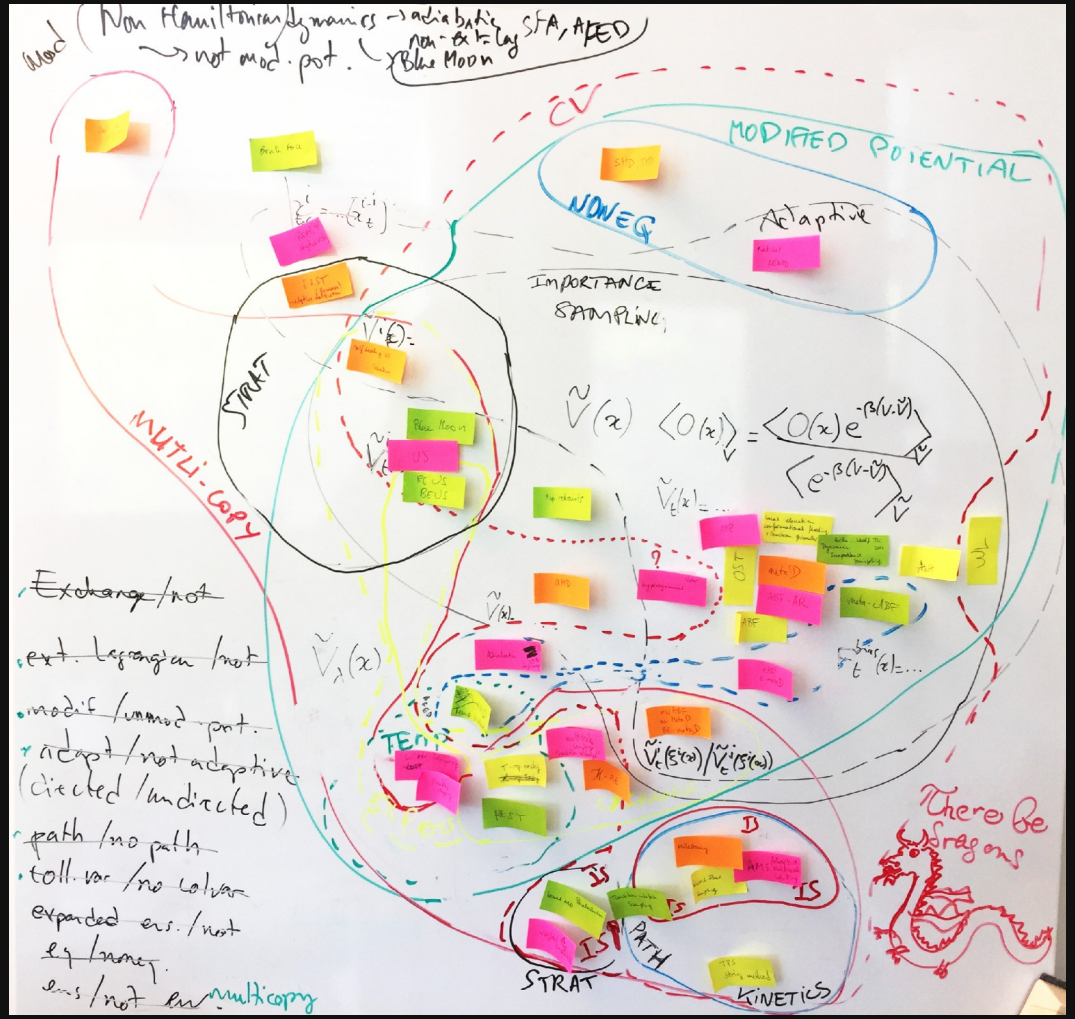
THE UNIVERSITY OF CHICAGO
PRITZKER SCHOOL OF MOLECULAR ENGINEERING



Pablo Zubieta

Argonne National Laboratory
October 13

MICCoM Workshop & Hands-on Tutorials 2022



Hénin, et al.
arXiv:2202.04164v1

Hardware acceleration

Enhanced sampling methods

Coarse-grained models

Enhanced Sampling Molecular Dynamics

Software Suite for Advanced
General Ensemble Simulations

PLUMED

Colvars

Limitations of existing solutions

Hard or cumbersome extensibility

They can be a computation bottleneck

Slow development or prototyping

Limitations of existing solutions

Lack of integration with standard ML libraries

There's a growing number enhanced sampling methods based on ML techniques

ANN
Sidky, Whitmer, 2018

FUNN
Guo, et al., 2018

CFF
Svegen, et al., 2020

MESA
Chen, Ferguson, 2018

PySAGES
Enhanced Sampling
MD on GPUs

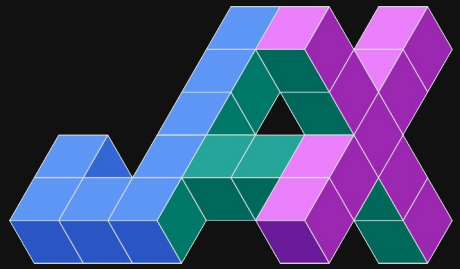
PySAGES features

Python interface

Ease for defining CVs and AD

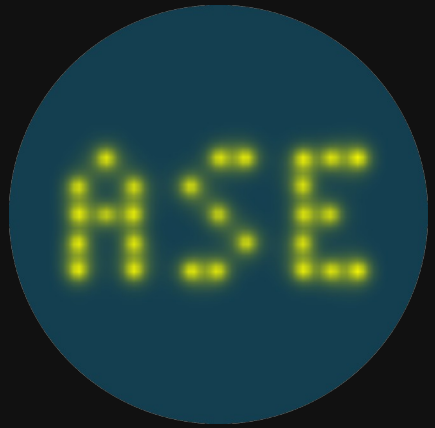
Machine learning libraries integration

Compute CVs and bias on the GPU

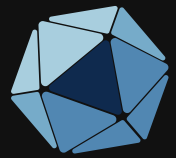


PySAGES features

Supported backends:



OpenMM



hoomdblue

PySAGES features

Sampling Methods:

Adaptive Biasing Force, Harmonic Biasing, Umbrella Sampling, Forward Flux Sampling, FUNN, ANN, MetaD, WTMetaD, String Method

Collective Variables:

Many “traditional” CVs have been implemented

PySAGES: Collective variables made easy

```python
class PerpendicularProjection(ThreePointCV):
    @property
    def function(self):
      return perpendicular

def perpendicular(p1, p2, p3):
    """
    Perpendicular projection of `p3` to the
    axis from `p1` to `p2`
    """
    r1 = barycenter(p1)
    r1 = barycenter(p2)
    r1 = barycenter(p3)
    a = r3 - r1
    b = r2 - r1
    return np.sqrt(np.dot(a, a) - np.dot(a, b)**2 / np.dot(b, b))
```

Parallel replicas Enhanced Sampling MD on GPUs

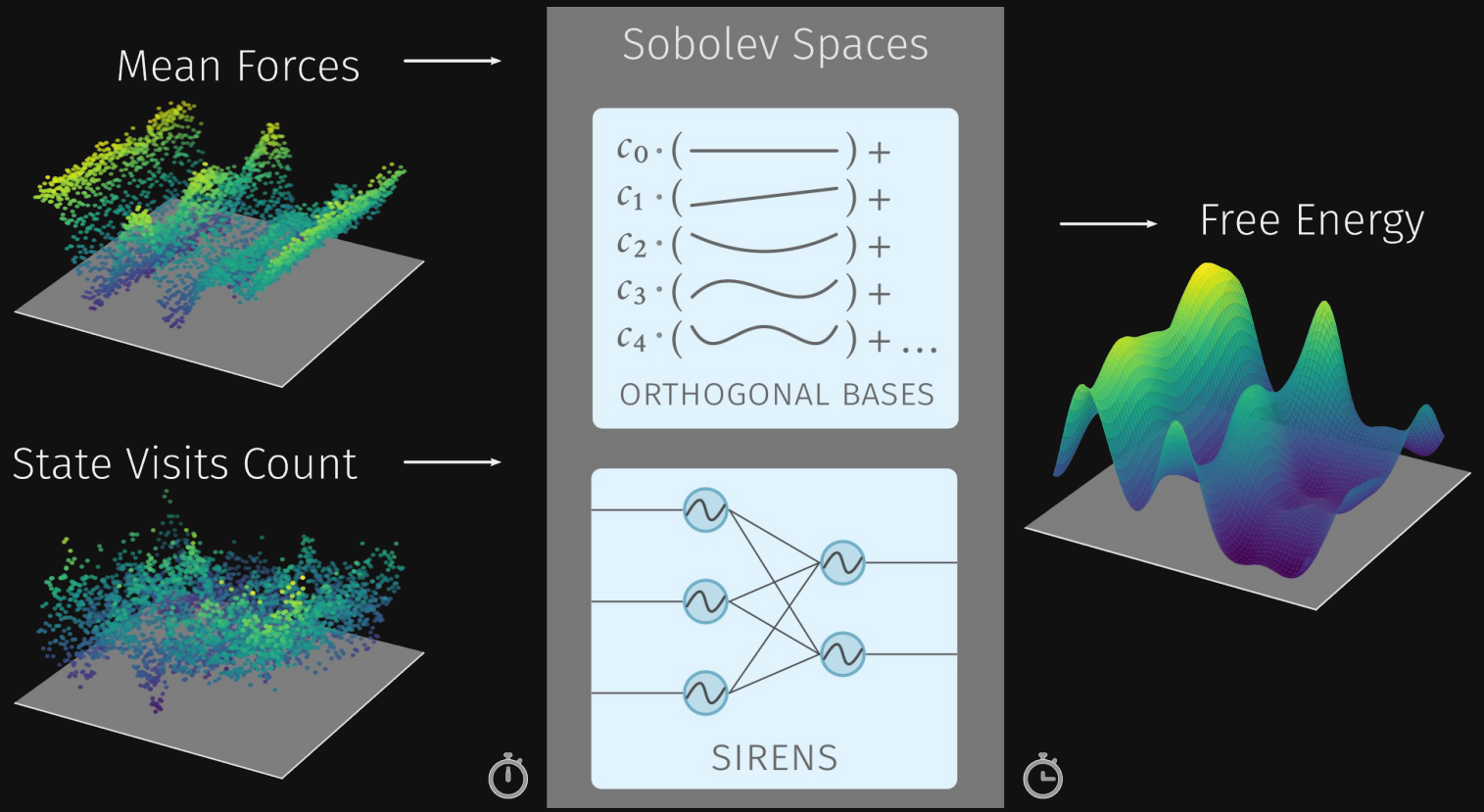
Analysis Tools

$$P_i^{\mathrm{u}}(\xi) = \frac{\int \exp[-\beta E(r)]\ \delta[\xi'(r) - \xi]\ d^N r}{\int \exp[-\beta E(r)]\ d^N r}.$$

$$A_i(\xi) = -(1/\beta)\ \ln P_i^{\mathrm{b}}(\xi) - w_i(\xi) + F_i.$$

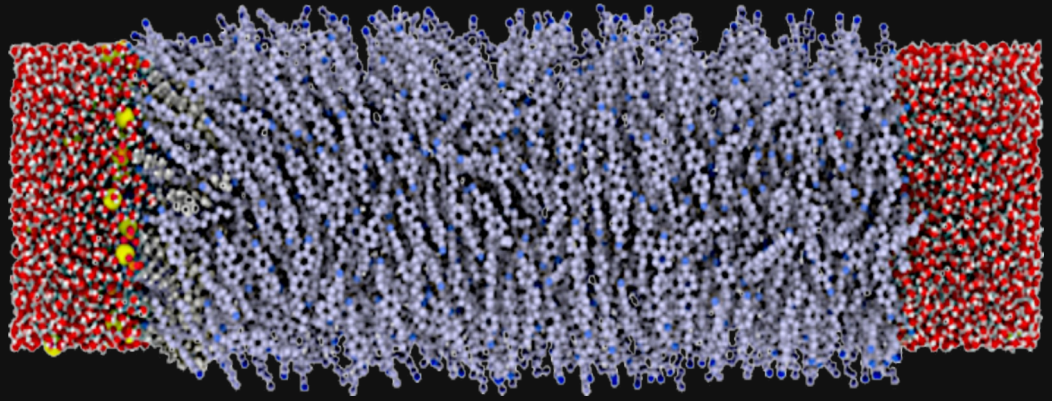
$$\frac{\partial A_i^{\mathrm{u}}}{\partial \xi} = -\frac{1}{\beta}\frac{\partial \ln P_i^{\mathrm{b}}(\xi)}{\partial \xi} - \frac{dw_i}{d\xi}.$$

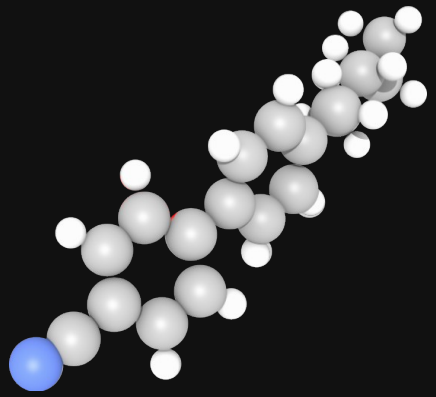
Fast sampling methods



https://doi.org/10.48550/arXiv.2202.01876

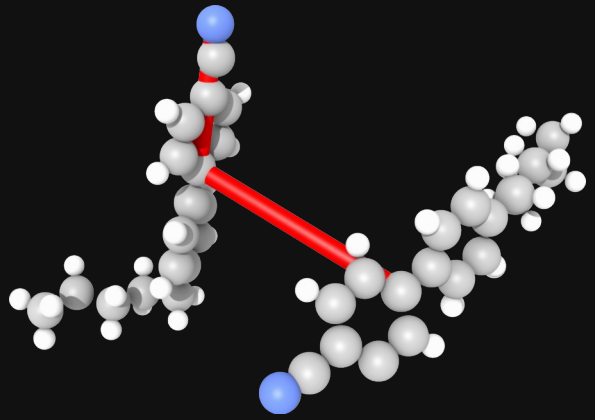
Use cases (Liquids Crystals)

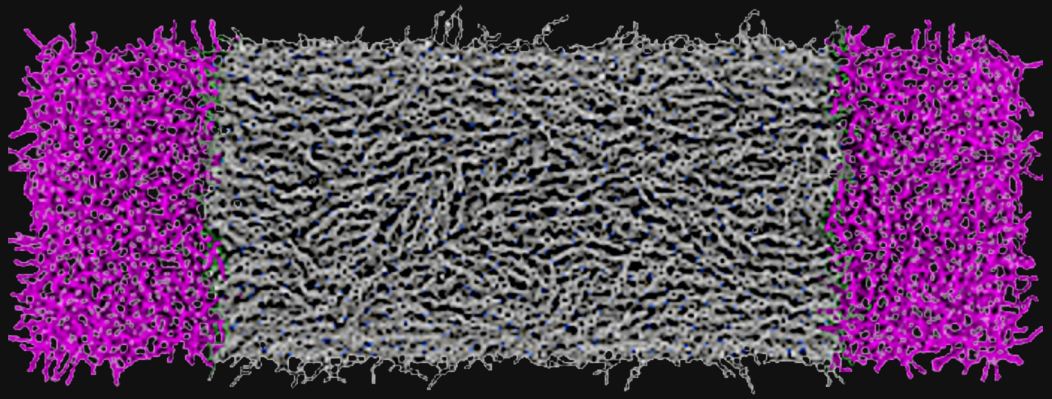




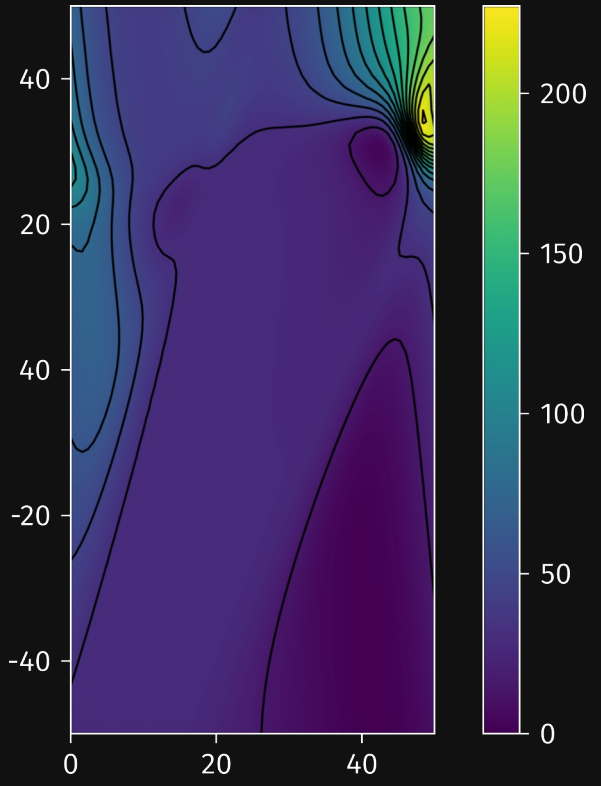
Gustavo Pérez-Lemus

Use cases (Liquids Crystals)

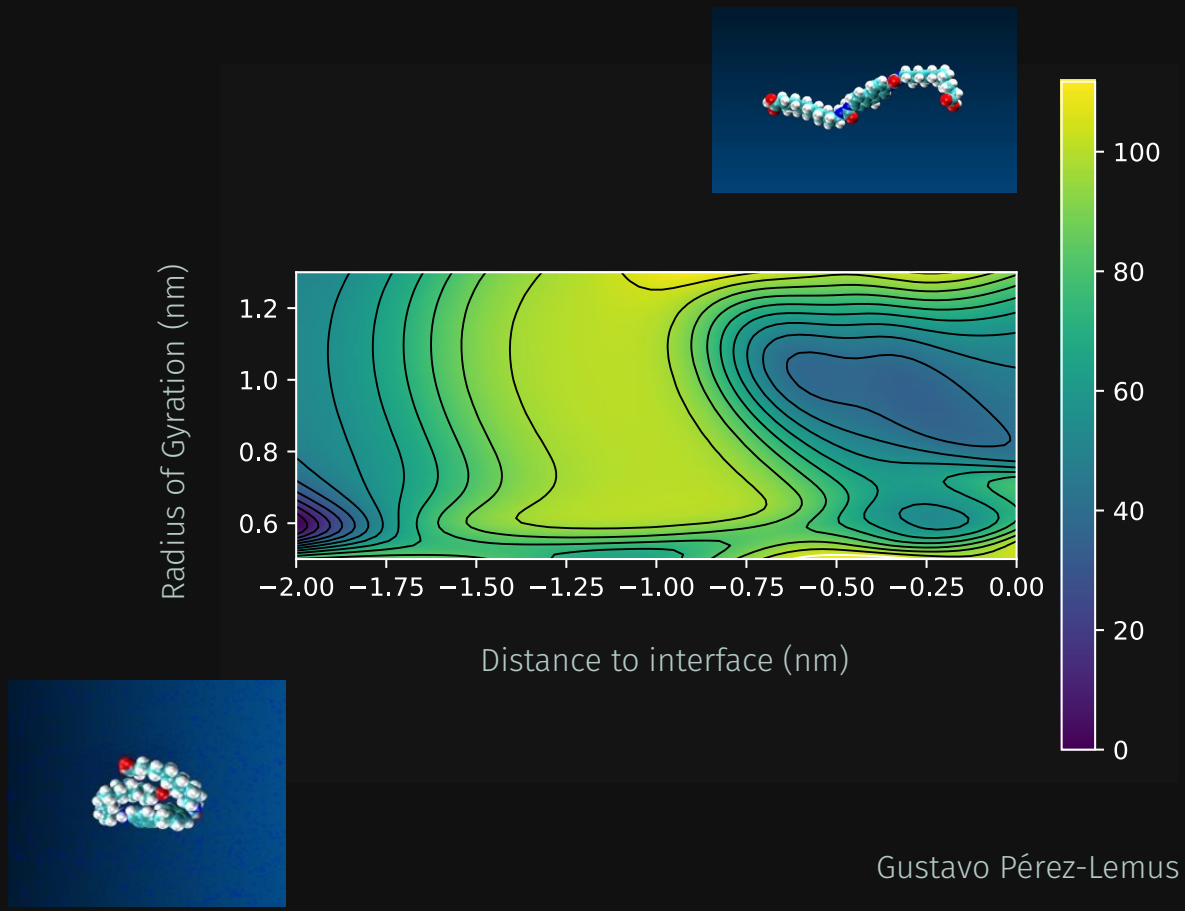




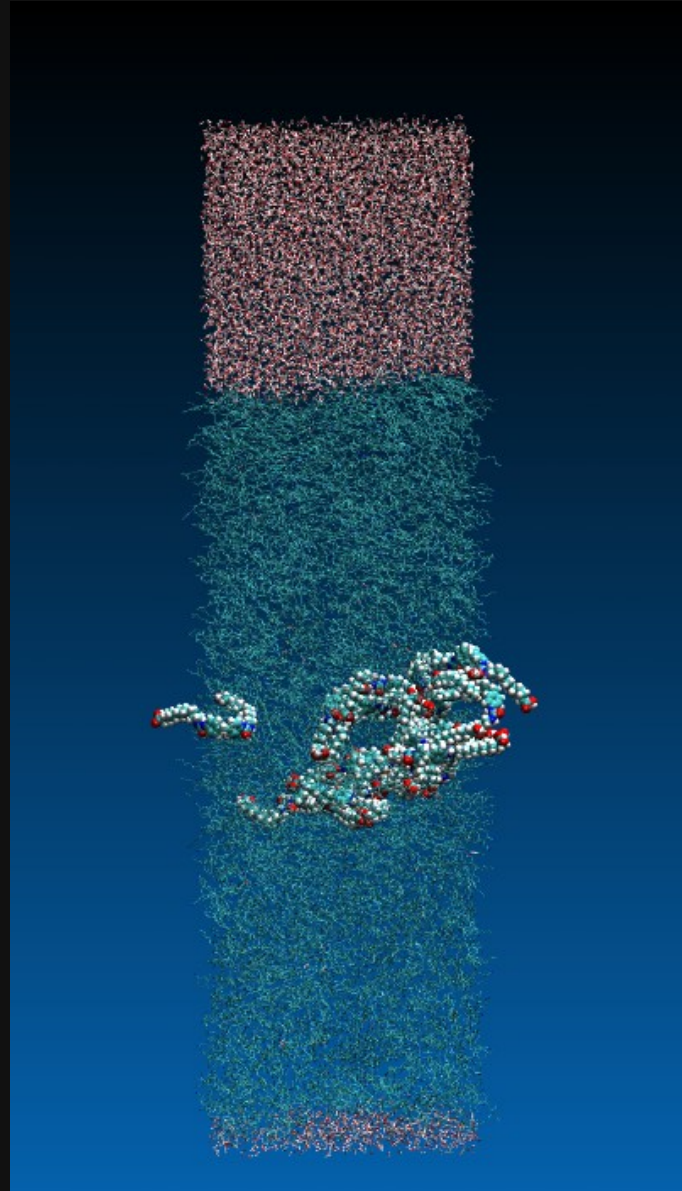
Gustavo Pérez-Lemus



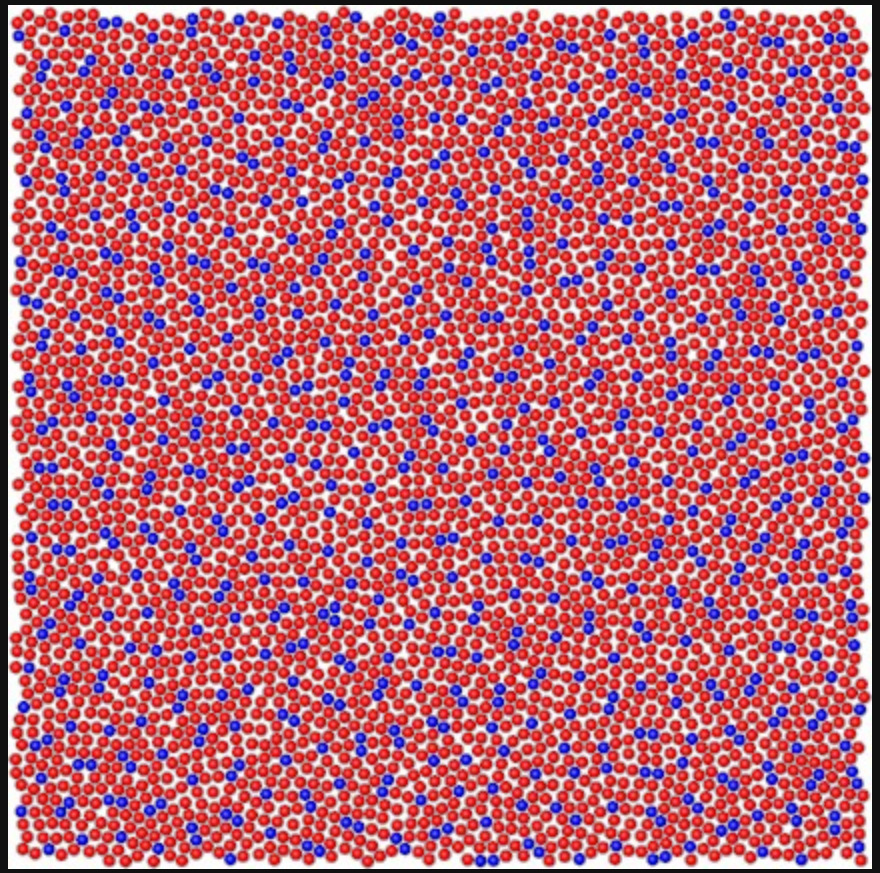
Use cases (Liquids Crystals)



Gustavo Pérez-Lemus

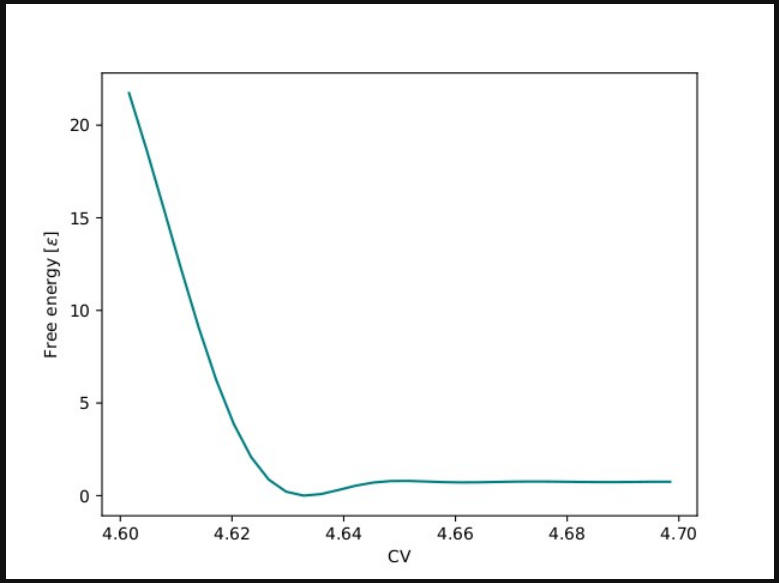


Use cases (Quasicrystals)



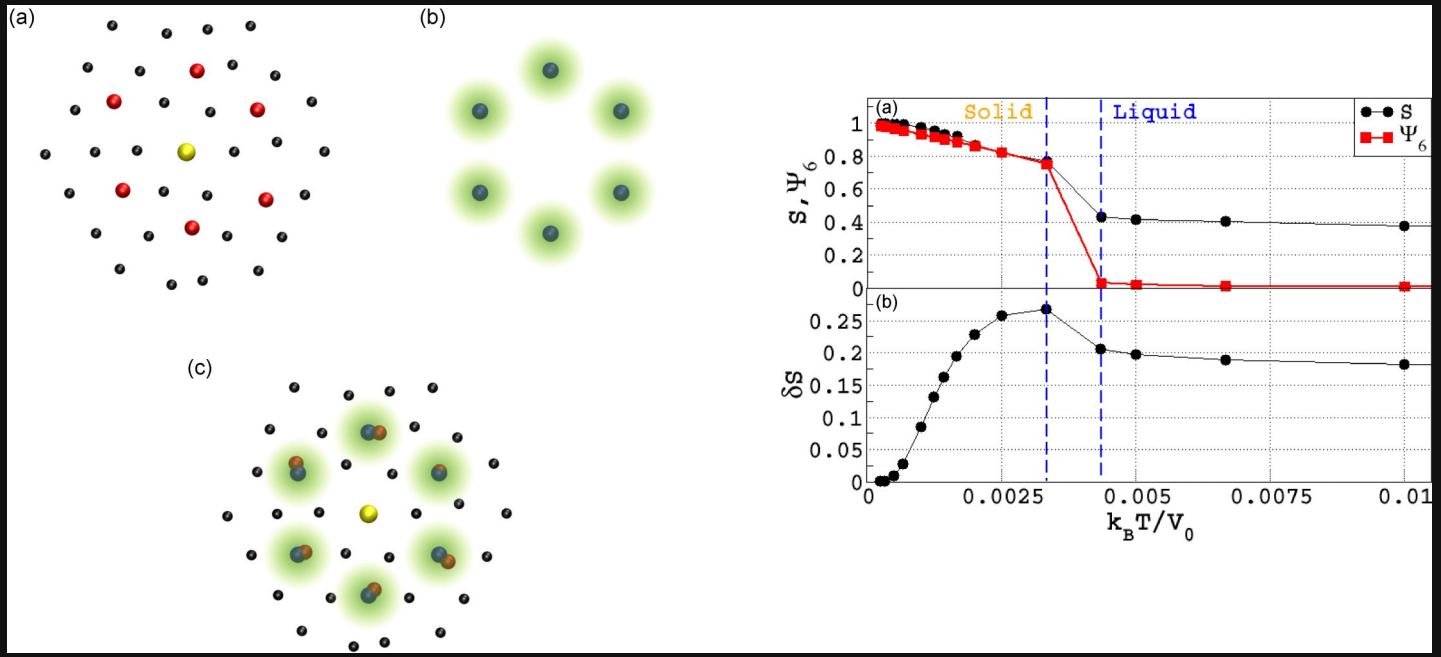
$$\xi = \sum_{i \in A} \sum_{i \in B} f_{ij}$$

$$s_{ij} = \frac{1 - \left(\frac{r_{ij} - d_0}{r_0}\right)^n}{1 - \left(\frac{r_{ij} - d_0}{r_0}\right)^m}.$$



Local Order Metric

$$\mathcal{O}(j)[\theta,\phi,\psi;\mathcal{P}] = \prod_{i=1}^{M} \exp\left(-\frac{\left|\mathbf{P}_{i_{\mathcal{P}}}^{j} - \mathbf{R}_{i}^{j}\right|^{2}}{2\sigma^{2}M}\right)$$



Martelli, et al.
10.1103/PhysRevB.97.064105

Current developments

Documentation

Nudge Elastic Band

CV discovery

Support more MD backends:
I-Pi, Qbox, LAMMPS, JAX-MD

Online tutorials

Easy to deploy PySAGES environments in Google Colab

https://github.com/SSAGESLabs/PySAGES/tree/main/examples

Find the code at

https://github.com/SSAGESLabs/PySAGES

Acknowledgements

Prof. Juan de Pablo

Ludwig Schneider
Gustavo Pérez-Lemus
John Parker (RCC)
Riccardo Alessandri
Siva Dasetty
(Ferguson group)
Trung Nguyen (RCC)

THE UNIVERSITY OF CHICAGO
PRITZKER SCHOOL OF MOLECULAR ENGINEERING

MICCoM