

# Probabilistic sampling for physics: finding needles in a field of high-dimensional haystacks

## Welcome Address

Organisation committee: Manon Michel (CNRS, Uni. Clermont-Auvergne), Thomas Swinburne (CNRS, Uni. Aix-Marseille)

Program manager: Francesca Sconfienza

Scientific committee: Alain Durmus (École Polytechnique), Virginie Ehrlacher (École des Ponts), Guilhem Lavaux (IAP), Mihai-Cosmin Marinica (CEA), Martin Weigel (Chemnitz Uni)

IPa Program

September, 4th - October, 22th 2023

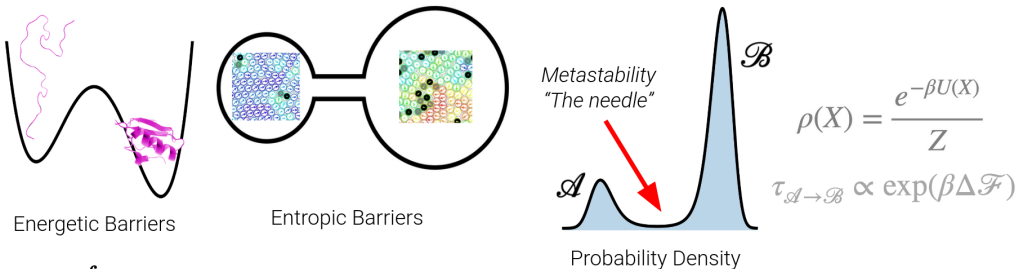


Claude Monet, Meules de foin, Fin de l'été (1891)



# Goals of the program

Distributions are often multimodal or sparse in high dimension

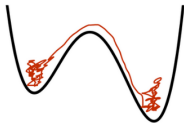


$$\rho(X) = \frac{e^{-\beta U(X)}}{Z}$$

$$\tau_{\mathcal{A} \rightarrow \mathcal{B}} \propto \exp(\beta \Delta \mathcal{F})$$

$$\langle O \rangle = \int \hat{O}(X) d\rho(X) \quad \text{Thermodynamic stability, transition kinetics, phase transition}$$

Standard strategy, Markov Chain Monte Carlo:  
Generate trajectories via **local** moves to explore,  
requires **exponentially large** number of moves



$$\langle O \rangle \simeq \lim_{N \rightarrow \infty} \sum_t \hat{O}(X_t)$$

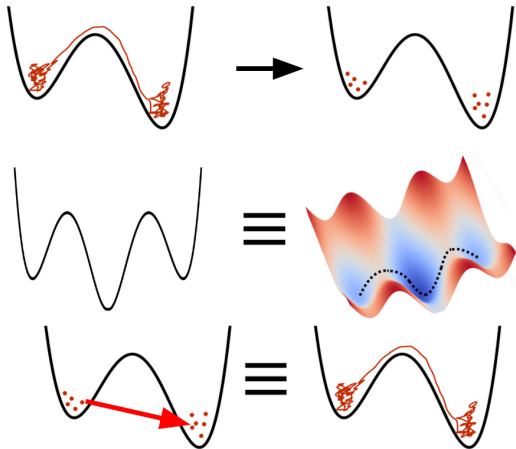
**Can we accelerate MCMC with advanced moves?**

**What physics can we preserve and extract along such dynamics?**

**How to build reduced representations that can detect previously unseen events or regions?**

# Goals of the program

- ▶ Can we accelerate MCMC with advanced moves? e.g.:
  - Generate non-local moves
  - Collective moves
  - Population annealing, histogram methods, nested sampling
  - Theoretical guarantees
- ▶ How to build reduced representations that can detect previously unseen events or regions? e.g.:
  - Generative models
  - Coarse-graining
  - Active learning
- ▶ What physics can we preserve and extract along such dynamics? e.g.:
  - Parallel-in-time methods
  - Dynamic accuracy in coarse-graining
  - Enhanced sampling



# Scientific program

## Presentations (open to all)

- ▶ Thematic sessions
- ▶ Colloquiums
- ▶ Faraday discussions
- ▶ Results communications

Hackathon sessions (only for participants)

Free collaboration

Local broadcast through zoom. A zoom recording and remote broadcast is planed, with speaker agreement.

## Brainstorming sessions (only for participants)

- ▶ Monday 4th: Metastability - chaired by Thomas Swinburne (thomas.swinburne@cnrs.fr)
- ▶ Tuesday 5th: Beyond random-walk behavior - chaired by Manon Michel (manon.michel@uca.fr)
- ▶ Wednesday 6th: Learning and sampling - chaired by Grant Rotskoff (rotskoff@stanford.edu)
- ▶ Thursday 7th: Preserving physics in dynamics - chaired by Pierre Monmarché (pierre.monmarche@sorbonne-universite.fr)
- ▶ Monday 11th: Enhanced sampling - chaired by Gabriel Stoltz (gabriel.stoltz@enpc.fr)
- ▶ Tuesday 12th: Mixing and convergence - chaired by Tim Garoni (tim.garoni@monash.edu)

# Hackathon

## Goal

To promote long-term and interdisciplinary collaborations, a focus of the afternoon sessions will be both the design and, importantly, implementation of benchmark problems for stochastic sampling. This will allow the relative strengths of available methods to be assessed in detail, and provide a concrete framework for collaborations.

## Example Systems

We have begun compiling a repository of example systems, simulated using Python and Julia MD libraries.

These are available at [github.com/tomswinburne/IPa\\_PSP\\_Hackathon/](https://github.com/tomswinburne/IPa_PSP_Hackathon/), and can be run online with Google colab (Google account required).

The systems are simple metastable models of atomic and spin systems. Thank you for your suggestions- more will be added during the week !

# Publications

## Cahiers de l'Institut Pascal

The achieved work (original results and review articles) will be featured as publications in Cahiers de l'Institut Pascal, published by EDP Sciences.

## Acknowledgment

"This work was made possible by Institut Pascal at Université Paris-Saclay with the support of the program "Investissements d'avenir" ANR-11-IDEX-0003-01 ".

# Workspace

## Talks at Amphitheatre

## Offices

Thomas and Manon can be found at the office near Cathedrale. For the vast majority, offices are floating. Do not worry there is room for all!

The offices have no garbage cans. So, please, in order to dispose of your waste, we thank you for using the selective sorting bins located in the corridors and for leaving your office clean when you leave.

Please note that lockable cabinets are available in all of the guest offices for you to secure your laptop and other valuables.

## Collaboration spaces

Cathedrale, Terrace, L107, L203, L217

## Remote access by zoom

Even possible at Cathedrale!

## Shared space

IPa also shares several facilities and communal rooms with 2 physics laboratories (FAST and LPTMS), including a library, a reception hall and a shower facility.

# Communication

- ▶ Mails
- ▶ Program website (abstracts, schedule):  
<https://indico.ijclab.in2p3.fr/event/9042/>
- ▶ Slack channel: Scientific discussion, slides/paper sharing, hackathon organisation, social activities organisation
- ▶ Thomas and Manon's office at Cathedrale



## Feedback

- ▶ Immediately after the program has ended, every invited attendee will receive a feedback survey via email, which they can complete anonymously.  
This survey contains questions about the scientific qualities of the program, as well as the logistical or administrative aspects.
- ▶ About one year after, another survey will normally be sent in order to assess how the program has impacted your research field and yielded fruitful outcomes (such as new collaborations, published articles, new research projects, fundings secured, etc.).

# Social activities

## Scheduled

- ▶ The two planned coffee/tea breaks are at Cathedrale, but feel free to help yourself anytime. The kitchenette includes coffee machines, a microwave, a refrigerator, and light refreshments are made readily available throughout the day.
- ▶ Monday lunch buffet is at Cathedrale. The lunch breaks of the other days are at the canteen, next to IPa.
- ▶ Social drinks are on Tuesday, on Terrace.
- ▶ Social dinner is on Thursday, you will be asked to answer an attendance poll on Slack beforehand.

## Free

- ▶ Plans for dinner on other days can be discussed on the slack channel *dinner-plans*.
- ▶ Plans for the weekend can be discussed on the slack channel *weekend-plans*.

# Life at IPa

- ▶ Program manager: Francesca Sconfienza, francesca.sconfienza@universite-paris-saclay.fr
- ▶ Participant guide:  
<https://www.institut-pascal.universite-paris-saclay.fr/sites/default/files/2022-06/Institut%20Pascal%20Guide%20for%20Participants.pdf>
- ▶ Access to the building: The door of the main entrance will generally be open between 9 am and 5 pm from Monday to Friday. If you need to access the building outside of these hours, please see with Francesca or Thomas and Manon.
- ▶ Wifi: For those that do not have access to Eduroam, visitor Wi-Fi logins will be provided by Francesca.
- ▶ If you do not wish to be on pictures, please do not be on picture!
- ▶ The offices have no garbage cans. Please dispose of your waste.
- ▶ Access to the IPa canteen: aim for 1 pm.