

Multi-canonical methods and lattice field theory

Report of Contributions

Contribution ID: 1

Type: **not specified**

Expanded Ensemble Method for Bubble Nucleation

Monday 1 December 2025 14:40 (40 minutes)

Many extensions of the Standard Model feature first-order phase transitions at the electroweak scale. These are particularly interesting since they may source gravitational waves, the spectrum of which is, in part, determined by the nucleation rate of bubbles. Computing this rate on the lattice requires us to determine the probability of the heavily suppressed critical bubble configurations.

While a standard application of the multicanonical method removes the obvious Boltzmann suppression, the condensation barrier is unaffected. This barrier appears at the condensation transition, which marks the point where the likely configuration changes from delocalised fluctuations of the metastable phase to a single localised bubble of the stable phase. The barrier increases with the system volume and causes exponential slowing down.

The ineffectiveness of the multicanonical method stems from the inability of the order parameter to distinguish fluctuations from small bubbles. In this talk, I will present an effective method for evading this deficiency, using expanded ensembles and non-homogeneous order parameters.

Special requests

Assuming acceptance, it would be preferable that the assigned timeslot would NOT be on Tuesday 2.12. before noon.

Author: HÄLLFORS, Jaakko (University of Helsinki)

Co-author: Prof. RUMMUKAINEN, Kari (University of Helsinki)

Presenter: HÄLLFORS, Jaakko (University of Helsinki)

Session Classification: Talks

Contribution ID: 2

Type: **not specified**

A canonical formulation of lattice QCD with physical quark masses

Monday 1 December 2025 16:00 (40 minutes)

QCD at finite temperature and density is usually studied in the lattice formalism with a grand canonical approach, where the properties of the system are defined in terms of the baryochemical potential μ . Studies in the canonical formulation are less common. Here we present first canonical results computed with physical quark masses. The simulations have been performed on $16^3 \times 8$ lattices using $2 + 1$ 4HEX improved staggered fermions.

We also present first results with both the strangeness (n_S) and baryon (n_B) densities as parameters. Specifically, we compute the QCD pressure and chemical potentials as functions of n_B and n_S and we are able to compare our results with Hadron Resonance Gas model.

Special requests

I would need to leave on Friday the 5th, would it be possible to speak before?

Authors: ADAM, Alexander (University of Wuppertal); BORSANYI, Szabolcs (University of Wuppertal); FODOR, Zoltan (Pennsylvania State University); GUENTHER, Jana (University of Wuppertal); PAROTTO, Paolo (University of Torino); PÁSZTOR, Attila (Eötvös Loránd University); PIRELLI, Ludovica (University of Wuppertal); WONG, Chik Him (University of Wuppertal)

Presenter: PIRELLI, Ludovica (University of Wuppertal)

Session Classification: Talks

Contribution ID: 3

Type: **not specified**

A scalable flow-based approach to mitigate topological freezing

Friday 5 December 2025 09:40 (40 minutes)

In recent years, flow-based samplers have emerged as a promising alternative to traditional sampling methods in lattice gauge theory. In this talk, we will introduce a class of flow-based samplers known as Stochastic Normalizing Flows (SNFs), which combine neural networks with non-equilibrium Monte Carlo algorithms. We will show that SNFs exhibit excellent scaling with the volume in lattice $SU(3)$ gauge theory. Then, we will present an application to $SU(3)$ gauge theory with open boundary conditions, demonstrating how this approach represents an efficient strategy for the sampling of topological observables at fine lattice spacings.

Special requests

Author: CELLINI, Elia (University of Edinburgh)

Co-authors: BONANNO, Claudio (IFT UAM/CSIC Madrid); BULGARELLI, Andrea (University of Bonn); NADA, Alessandro (University of Turin and INFN Turin); PANFALONE, Dario (University of Turin and INFN Turin); VADACCHINO, Davide (University of Plymouth); VERZICHELLI, Lorenzo (University of Turin and INFN Turin)

Presenter: CELLINI, Elia (University of Edinburgh)

Session Classification: Talks

Contribution ID: 4

Type: **not specified**

Monte Carlo methods for data mining in complex systems.

Friday 5 December 2025 11:40 (40 minutes)

Many complex systems are modular. Such systems can be represented as “component systems”, i.e., sets of elementary components, such as proteins in cells or neurons in the brain. These systems are strongly constrained but the underlying functional design and architecture (for example the structure of gene-regulatory interactions in the cell) is not obvious a priori, and its detection is often a challenge of both scientific and practical importance, requiring a clear understanding of component statistics. In this talk I will discuss a set of tools based on a hierarchical version of Stochastic Block Modeling (hSBM) which allow to infer the functional modules of such systems. These algorithms are based on the minimization of an information-theoretic quantity known as “description length” which behaves in many respects as the free energy of a statistical mechanics model and can be explored using algorithms similar to those adopted in more standard statistical mechanics problems.

Special requests

I will only be arriving on Tuesday evening, so I would kindly ask that my talk be scheduled on one of the final three days of the workshop.

Author: CASELLE, Michele (Università di Torino)

Presenter: CASELLE, Michele (Università di Torino)

Session Classification: Talks

Contribution ID: 5

Type: **not specified**

Energy-based diffusion models for complex actions

Wednesday 3 December 2025 09:00 (40 minutes)

Energy-based diffusion models can learn the unnormalised probability distribution from data. We apply this idea to a well-studied example in the context of lattice field theories with a sign problem, for which training data is generated using complex Langevin dynamics. We demonstrate that the learned distribution can subsequently be used to generate configurations using importance sampling. This final (i.e., after training) generative step therefore bypasses both complex Langevin and diffusion model dynamics.

Special requests

Author: AARTS, Gert (Swansea University and ECT*)

Presenter: AARTS, Gert (Swansea University and ECT*)

Session Classification: Talks

Contribution ID: 7

Type: **not specified**

SU(N) eigenstates with Physics-Informed Neural Networks

Friday 5 December 2025 11:00 (40 minutes)

We propose a novel algorithm for the solution of the Schrödinger equation of SU(N) lattice gauge theories. Physics-Informed Neural Networks (PINNs) are employed to find the coupling flow of the eigenstates, starting from the strong coupling limit and evolving adiabatically towards the continuum limit at $1/g \rightarrow \infty$. For each strong-coupling eigenstate, the trained network provides a representation of the wavefunction, and during the training also its energy is learned as a parameter.

Special requests

Author: Dr ROMITI, Simone (Uni-Bern)

Presenter: Dr ROMITI, Simone (Uni-Bern)

Session Classification: Talks

Contribution ID: 8

Type: **not specified**

Applying normalising-flow-based density of states to 2D U(1) lattice gauge theory with a θ -term

Monday 1 December 2025 11:40 (40 minutes)

The normalising-flow-based density of states approach has recently been shown to successfully reconstruct the partition function of (1+1)D scalar field theories, recovering the correct Lee–Yang zeros. In this talk, we extend this idea by applying gauge-equivariant normalizing flows to reconstruct the density of states in pure (1+1)D U(1) gauge theory with a θ -term. In particular, we focus on the steps required to probe the topological phase transition expected at $\theta = \pi$.

Special requests

Author: SINGH, Simran (University of Bonn)

Presenter: SINGH, Simran (University of Bonn)

Session Classification: Talks

Contribution ID: 9

Type: **not specified**

Implications of Yukawa interactions in scalar sector

Tuesday 2 December 2025 14:40 (40 minutes)

In this work, a field theory model containing a real scalar singlet and an $SU(2)$ symmetry preserving complex doublet is studied using the method of lattice simulations. The model considers all quartic vertices along with the Yukawa vertex between a real scalar singlet and an $SU(2)$ symmetry preserving complex doublet field. Machine learning is used to extract representative functions of the field propagators, lattice regulator, and the Yukawa vertex. In the considered renormalization scheme the field propagators are found enhanced compared to their respective tree level structure. It is found that mixing of operators containing scalar singlet with $SU(2)$ invariant field operators results in 0

+ states with a peculiar scarcity in hundreds of GeV s. The Yukawa vertex shows weak dependence on the field momenta while the theory remain interactive as found by the renormalized field propagators. The impact of the real scalar quartic self interaction is found mitigated due to other interaction vertices. The field expectation values exhibit a certain classification despite no conclusive signal of phase transition.

Special requests

Authors: SAAD, Muhammad (LUMS); Dr MUFTI, Tajdar (LUMS)

Presenter: SAAD, Muhammad (LUMS)

Session Classification: Talks

Contribution ID: 10

Type: **not specified**

Free energy difference with Jarzynski equality: Interfaces in the lattice ϕ^4 theory

Friday 5 December 2025 09:00 (40 minutes)

Jarzynski equality allows the determination of the free energy difference between the initial and final macrostate of the out-of-equilibrium evolution of a thermodynamic system. This notion has recently been applied to out-of-equilibrium Markov chain Monte Carlo simulations of lattice field theories. The main goal of this talk is to illustrate this methodology.

In particular, we employ this method to study the lattice ϕ^4 theory, in three dimensions. We tune the parameters of the theory so that the $\mathbb{Z}_2$ symmetry is spontaneously broken, but close to the critical line. In this setup, we study the free energy difference between the periodic and anti-periodic boundary conditions, which can be directly accessed thanks to the Jarzynski equality.

Depending on the geometry of the lattice, the free energy difference can be interpreted in terms of an effective string theory describing an interface between the two vacua with opposite spontaneous magnetization. We point out the deviations from the free boson behavior and even hints of deviations from the Nambu-Goto string prediction.

Special requests

Authors: Dr NADA, Alessandro (Università di Torino, INFN sezione di Torino); Dr CELLINI, Elia (University of Edinburgh); VERZICHELLI, Lorenzo (Università di Torino, INFN sezione di Torino); Prof. CASELLE, Michele (Università di Torino, INFN sezione di Torino); Mr CHIAPASCO, Umberto (Università di Torino)

Presenter: VERZICHELLI, Lorenzo (Università di Torino, INFN sezione di Torino)

Session Classification: Talks

Contribution ID: 11

Type: **not specified**

The smeared R-ratio in isoQCD from first-principles lattice simulations

Tuesday 2 December 2025 14:00 (40 minutes)

The R-ratio is a phenomenological observable of great relevance, both in itself and in applications such as the dispersive approach to the muon anomalous magnetic moment. It can be investigated from first-principles in lattice QCD by introducing an arbitrary smearing kernel and employing the well-known Hansen-Lupo-Tantalo method to perform spectral reconstruction with controlled statistical and systematic errors. Improving upon a first study published in 2023, we show preliminary results using the correlation functions produced by ETMC in $N_f = 2 + 1 + 1$ lattice simulations at four lattice spacings, different volumes and with higher statistics w.r.t. our previous study. The new correlators, thanks to the implementation of the Low Mode Average technique, allow the determination of the R-ratio smeared with Gaussian kernels of widths down to $\sigma \sim 200$ MeV with phenomenologically relevant precision.

Special requests

Author: MARGARI, Francesca**Presenter:** MARGARI, Francesca**Session Classification:** Talks

Contribution ID: 12

Type: **not specified**

Fighting topological freezing in $SU(N)$ Yang–Mills theories with the PTBC algorithm

Thursday 4 December 2025 11:40 (40 minutes)

We discuss two applications of the Parallel Tempering on Boundary Conditions (PTBC) algorithm to fight topological freezing in the simulation of $SU(N)$ Yang–Mills theories on the lattice: the determination of the renormalized coupling in the Twisted Gradient Flow scheme and the scale setting via gradient flow. We show that the PTBC algorithm is much more efficient in decorrelating the topological charge compared to standard algorithms, largely reducing statistical uncertainties at same computational effort. Also, it allows not to rely on the projection to the trivial topological sector, used as a workaround to topological freezing, thus avoiding the power-like finite-volume corrections arising from a fixed topology. Moreover, we discuss an implementation of the Multi-canonical Monte Carlo method to improve the efficiency of the PTBC algorithm when topological modes are highly suppressed.

Special requests

Authors: Dr BONANNO, Claudio (Istituto de Fisica Teorica (IFT), UAM/CSIC); Prof. D’ELIA, Massimo (Dipartimento di Fisica “E. Fermi”, Università di Pisa); GIORGIERI, Andrea (University of Pisa); Dr GARCÍA PÉREZ, Margarita (Istituto de Fisica Teorica (IFT), UAM/CSIC); Dr DASILVA GOLÁN, Jorge Luis (Brookhaven National Laboratory (BNL))

Presenter: GIORGIERI, Andrea (University of Pisa)

Session Classification: Talks

Contribution ID: 13

Type: **not specified**

Variance reduction with machine-learned flows

Tuesday 2 December 2025 09:00 (40 minutes)

We present an application of machine-learned flows that reduces the variance in lattice QCD observables. This approach is effective when the desired observable or correlation function can be expressed as a derivative with respect to an action parameter. We demonstrate the computational advantage of this method for several quantities in pure-gauge SU(3) and QCD.

Special requests

Author: ROMERO-LOPEZ, Fernando (Uni Bern)

Presenter: ROMERO-LOPEZ, Fernando (Uni Bern)

Session Classification: Talks

Contribution ID: 14

Type: **not specified**

The density of states in finite-temperature $Sp(4)$ Yang-Mills theory

Monday 1 December 2025 11:00 (40 minutes)

Sampling methods based on the density of states provide a framework for determining properties of first-order phase transitions of gauge theories from first principles. These transitions are physically interesting, e.g. in the context of predicting a stochastic gravitational wave signal from early universe phase transitions. I will present results for $Sp(4)$ Yang-Mills theory around its first-order thermal phase transition by reconstructing the density of states via the logarithmic linear relaxation (LLR) algorithm. I will show results on different space and time extents, as well as aspect ratios, and estimate discretisation artifacts. We see clear signatures of the first-order transition and determine the critical coupling, the specific heat and set bounds on the surface tension.

Special requests

It would be great if this talk takes place after the one from David Mason

Author: ZIERLER, Fabian (Technical University of Munich)

Co-authors: LUCINI, Biagio; MASON, David; VADACCHINO, Davide; BENNETT, Ed; RINALDI, Enrico; PIALI, Maurizio

Presenter: ZIERLER, Fabian (Technical University of Munich)

Session Classification: Talks

Contribution ID: 15

Type: **not specified**

Logarithmic linear relaxation method for non-Abelian gauge theories at finite temperature

Monday 1 December 2025 09:40 (40 minutes)

The logarithmic linear relaxation (LLR) method is a density of states method that can precisely determine thermodynamic properties of first order phase transitions, by analysing the micro-canonical structure of both the stable and meta-stable branches of the transition. This method has become particularly interesting in the context of first order confinement transitions at finite temperature in beyond the standard model physics, due to potential links to gravitational wave physics through bubble nucleation in the meta-stable vacuum. In this contribution I will discuss the algorithmic details of our collaborations implementation of the LLR method and discuss possible future directions.

Special requests

If possible could I please speak before Fabian Zierler

Author: MASON, David (Jülich Forschungszentrum)

Co-authors: Prof. LUCINI, Biagio (Queen Mary University of London); Dr VADACCHINO, Davide (University of Plymouth); Dr BENNETT, Ed (Swansea University); Dr RINALDI, Enrico; Dr ZIERLER, Fabian (Technical University of München); Prof. PIAI, Maurizio (Swansea University)

Presenter: MASON, David (Jülich Forschungszentrum)

Session Classification: Talks

Contribution ID: 16

Type: **not specified**

Exploration of parallel tempering to reduce topological freezing

Thursday 4 December 2025 14:00 (40 minutes)

In Lattice QCD, the problem of topological freezing refers to the increasingly long autocorrelation times of topological observables as the continuum limit is approached. In this talk, we present an analysis of a method known to mitigate this: *parallel tempering on boundary conditions*. This algorithm consists of simultaneously generating several Markov chains or “replicas”, each of these differing only by some condition on a subset of links of the lattice, and proposing an exchange between pairs of replicas through an accept/reject step. Based on this analysis, we also discuss under which conditions could this algorithm present a computational advantage on $SU(3)$ pure-gauge theory calculations.

Special requests

Author: GRANADOS PINTO, Victor Manuel (Universität Bern)

Presenter: GRANADOS PINTO, Victor Manuel (Universität Bern)

Session Classification: Talks

Contribution ID: 17

Type: **not specified**

Diffusion models for U(2) and SU(2) lattice field theory

Wednesday 3 December 2025 09:40 (40 minutes)

Recent works have shown diffusion models to be promising candidates for improving upon Monte Carlo methods in the context of lattice field theory. While these works have mostly focused on abelian groups, an application to QCD requires the extension to non-abelian gauge groups.

In this work, we consider U(2) and SU(2) lattice field theory, and further explore the extension of the method to U(3) and SU(3).

For generating field configurations, instead of the usual diffusion model sampling, we use the Metropolis-adjusted annealed Langevin scheme.

This may enable us to use a model which was trained at a specific coupling to extrapolate to stronger couplings where the usual Monte Carlo methods face problems.

Special requests

I think I mentioned it before, but please schedule my talk between monday and thursday, as I already have to leave on friday. Thank you! Thomas

Author: RANNER, Thomas (TU Wien)

Co-authors: Dr IPP, Andreas (TU Wien); Dr MÜLLER, David (TU Wien); Prof. AARTS, Gert (Swansea University); Dr WANG, Lingxiao (RIKEN); ZHU, Qianteng (INPAC, RIKEN); Prof. WANG, Wei (INPAC, SCNT)

Presenter: RANNER, Thomas (TU Wien)

Session Classification: Talks

Contribution ID: **18**Type: **not specified**

Results for fermionic observables by using a two-level sampling method

Tuesday 2 December 2025 11:00 (40 minutes)

I will discuss our recent work on using a two-level sampling algorithm in combination with distillation techniques for the computation of fermionic observables. Using a 1D decomposition of the lattice into two active domains separated by smaller frozen domain, the quark propagator can be written as a series of domain-local contributions. These contributions can be estimated independently with a two-level sampling strategy. This potentially enables an exponential gain in the signal-to-noise of fermionic correlators as the number of submeasurements increases. In the talk I will show our test results using a pure gauge ensemble. Here, we computed both the leading contribution and the first order terms in the measurements of disconnected diagrams.

Special requests

Authors: Dr FINKENRATH, Jacob; BARCA, Lorenzo; SCHAEFER, Stefan

Presenter: Dr FINKENRATH, Jacob

Session Classification: Talks

Contribution ID: 19

Type: **not specified**

The QCD Sphaleron Rate: A First-Principles Determination from Inverse-Problem Techniques

Tuesday 2 December 2025 11:40 (40 minutes)

The sphaleron rate is a key phenomenological quantity, relevant both for axion thermal production in the early Universe and for transport phenomena such as the Chiral Magnetic Effect.

I will begin by outlining the numerical strategy used to extract the sphaleron rate from lattice correlators, employing a regularized Backus–Gilbert reconstruction.

Then, I will present early results for the sphaleron rate at non-zero spatial momentum in pure-gauge theory, obtained from correlators double-extrapolated to the continuum and to zero smoothing radius.

Special requests

Authors: VALENTINO, Alessandra (Università di Pisa); Dr GIORGIERI, Andrea (Università di Pisa); Dr BONANNO, Claudio (IFT UAM/CSIC Madrid); Dr SANFILIPPO, Francesco (INFN, Sezione di Roma Tre); Dr GAGLIARDI, Giuseppe (Dipartimento di Matematica e Fisica, Università “Roma Tre”); Prof. D’ELIA, Massimo (Università di Pisa); DIONISIO, Roberto (Università di Pisa / INFN sez. di Pisa)

Presenter: DIONISIO, Roberto (Università di Pisa / INFN sez. di Pisa)

Session Classification: Talks

Contribution ID: 20

Type: **not specified**

Enhanced sampling methods to mitigate topological freezing

Thursday 4 December 2025 11:00 (40 minutes)

In lattice field theories with topological sectors, such as QCD and four-dimensional $SU(N)$ gauge theories with periodic boundary conditions, conventional update algorithms struggle to sample the whole configuration space due to large action barriers separating distinct topological sectors. This manifests itself in the form of long autocorrelation times that diverge in the continuum limit and can compromise the correctness of simulations.

Here, we demonstrate that with suitably constructed bias potentials, Metadynamics and related enhanced sampling methods can mitigate this problem and significantly reduce the integrated autocorrelation times of the topological charge and associated observables. In addition, we show how combining a biased and an unbiased simulation stream in a parallel tempering setup allows us to obtain unbiased expectation values without the need to perform any reweighting.

Special requests

Authors: HOELBLING, Christian (University of Wuppertal); FUWA, Gianluca (University of Wuppertal); EICHHORN, Timo (University of Wuppertal)

Presenter: EICHHORN, Timo (University of Wuppertal)

Session Classification: Talks

Contribution ID: 21

Type: **not specified**

Studying critical slowing down of topological observables

In this work, we focus on the development of algorithms to update the field configurations for lattice gauge theories. In particular, we have been interested in testing these methods using the CP^{N-1} model, which reproduces the same physical properties contained in QCD, such as asymptotic freedom, confinement and mass gap. This model has the advantage of being simpler to simulate (requires less computational cost), and therefore is a good laboratory for testing new methods.

We are going to discuss the main features of the simulations of the CP^{N-1} model, starting from the standard Monte Carlo techniques and going to the new possible perspectives. It can also be interesting to discuss whether these new ideas can be implemented in an efficient way to other cases of physical interest, such as gauge fixing.

Special requests

Author: KÜL, João Octavio (Universidade de São Paulo / University of Edinburgh)

Presenter: KÜL, João Octavio (Universidade de São Paulo / University of Edinburgh)

Session Classification: Talks

Contribution ID: 22

Type: **not specified**

Nested sampling for gauge theories

Thursday 4 December 2025 09:00 (40 minutes)

We consider nested sampling as a generic integration technique over the space of lattice gauge configurations. We discuss its advantages in cases where standard simulations are inefficient due to suppressed tunneling between (metastable) states. For example, nested sampling has the potential to overcome topological freezing in simulations at fine lattice spacings and we demonstrate this in the 2D U(1) gauge theory. Another example concerns first order phase transitions where nested sampling can be used to efficiently obtain the density of states. As an example we apply it to the deconfinement transition in the 4d SU(3) gauge theory.

Special requests

I'm participating only Wednesday and Thursday.

Author: WENGER, Urs

Co-authors: KANWAR, Gurtej; ROMITI, Simone

Presenter: WENGER, Urs

Session Classification: Talks

Contribution ID: 23

Type: **not specified**

Machine learning a fixed-point action for the $O(3)$ non-linear sigma-model in $d=2$

Wednesday 3 December 2025 11:40 (40 minutes)

In this talk, I present our results for the machine learning of a renormalization-group improved action for the $O(3)$ non-linear sigma-model in $d=2$. After introducing the theoretical setup, I will discuss the convolutional neural networks used in this study. Using these networks, we trained a neural network to parameterize a fixed-point action, a classically perfect action. Its properties are tested and it is compared to previously found parametrizations. Finally, I will conclude with an outlook on the conceptual steps needed for constructing a quantum perfect action for this theory.

Special requests

Author: BACKFRIED, Liane (Universität Bern)

Co-authors: IPP, Andreas; MÜLLER, David; WENGER, Urs

Presenter: BACKFRIED, Liane (Universität Bern)

Session Classification: Talks

Contribution ID: 24

Type: **not specified**

Equivariant Diffusion-based Sampling for Lattice Field Theory

Wednesday 3 December 2025 11:00 (40 minutes)

Recent advances in deep generative modeling have enabled accelerated approaches to sampling complicated probability distributions. In this work, we develop symmetry-equivariant diffusion models to generate lattice field configurations. We build score networks that are equivariant to a range of group transformations and train them using an augmented score matching scheme. By reweighting generated samples, we produce unbiased estimates for observables in scalar ϕ^4 theory and $U(1)$ gauge theory. We extend our framework to sample $SU(N)$ degrees of freedom by adapting the score matching technique and the reverse diffusion process to the group manifolds. Our trained models faithfully reproduce the target densities for several toy $SU(2)$ theories, which marks a step towards simulating full $SU(N)$ gauge theory on the lattice.

Special requests

Author: VEGA, Octavio (University of Illinois Urbana-Champaign)

Co-authors: Prof. KANWAR, Gurtej (University of Edinburgh); Dr KOMIJANI, Javad (ETH Zürich); Prof. MARINKOVIC, Marina (ETH Zürich); Prof. EL-KHADRA, Aida (University of Illinois Urbana-Champaign)

Presenter: VEGA, Octavio (University of Illinois Urbana-Champaign)

Session Classification: Talks

Contribution ID: 25

Type: **not specified**

Continuous normalizing flows for the quantum rotor

Wednesday 3 December 2025 14:00 (40 minutes)

In this talk I will discuss continuous normalizing flows for the sampling of the theory of quantum rotor. Using this toy model, we study the capability of continuous normalizing flows to sample across different topological sectors, and to help reduce noise in the computation of correlation functions.

Special requests

Author: CHENG, Miranda C.N. (U. Amsterdam and Academia Sinica, Taiwan)

Presenter: CHENG, Miranda C.N. (U. Amsterdam and Academia Sinica, Taiwan)

Session Classification: Talks

Contribution ID: 26

Type: **not specified**

Accelerating Parallel Tempering with Neural Transports

Thursday 4 December 2025 14:40 (40 minutes)

Markov Chain Monte Carlo (MCMC) is a powerful algorithmic framework for sampling from complex probability distributions. Standard MCMC methods struggle with high-dimensional distributions containing well-separated modes, becoming trapped in local regions. Parallel tempering (PT) addresses this by using intermediate annealing distributions to bridge a tractable reference (e.g., Gaussian) and an intractable target distribution. However, classical PT is inflexible, fragile, challenging to tune, and suffers from performance collapse for challenging inference tasks.

This talk introduces non-reversible parallel tempering (NRPT), which provably dominates classical reversible PT algorithms. We show that NRPT undergoes a sharp algorithmic phase transition with increased parallelism, where it becomes robust, easy to tune, and scales efficiently to GPUs. I will then demonstrate how to further accelerate PT using neural transports such as normalising flows and diffusions. We demonstrate this framework across a variety of examples in Bayesian inference and inference-time control for diffusion models, and discuss recent applications to cancer genomics and the Event Horizon Telescope.

Special requests

Author: SYED, Saifuddin (University of British Columbia)

Presenter: SYED, Saifuddin (University of British Columbia)

Session Classification: Talks

Contribution ID: 27

Type: **not specified**

Tackling the Signal to Noise problem with Stochastic Automatic Differentiation

Tuesday 2 December 2025 09:40 (40 minutes)

Lattice field theory allows for the direct computation of physical quantities in strongly coupled theories. In particular, numerical Monte Carlo simulations using Euclidean correlation functions give direct access to the energy spectrum of the theory. However, the fast degradation of the signal with the Euclidean time, known as the signal to noise problem, significantly affects the precision of such computations. A possible solution to the problem can be found by expressing the Euclidean correlators as derivatives with respect to sources in the action. Following this, two methods are presented, one as an extension of reweighting methods, and another inspired in the ideas of numerical stochastic perturbation theory. Both approaches involve the concept of Automatic Differentiation, which requires an extension to stochastic processes, in particular for its use in Monte Carlo simulations. Results will be shown in a four-dimensional scalar theory.

Special requests

Author: CATUMBA, Guilherme (University Milano-Bicocca)

Presenter: CATUMBA, Guilherme (University Milano-Bicocca)

Session Classification: Talks

Contribution ID: 28

Type: **not specified**

Revisiting collective-variable guided sampling with normalizing flows

Wednesday 3 December 2025 14:40 (40 minutes)

Deep generative models parametrize very flexible families of distributions able to fit complicated datasets of images or text. These models provide independent samples from complex high-distributions at negligible costs. On the other hand, sampling exactly a target distribution, such as the Boltzmann distribution of a physical system, is typically challenging: either because of dimensionality, multi-modality, ill-conditioning or a combination of the previous. A recent line of work using generative models to accelerate sampling has shown promises but still struggles as the system size gets large. In this talk, I will discuss an approach tackling this challenge by using a generative model to explore the configuration space of a collective-variable (CV) and a non-equilibrium candidate Monte Carlo to recover an unbiased all-atoms configurations. The approach revisits CV-guided sampling with two main advantages. Firstly, the collection of CVs need not be restricted to a few variables and can include tens or hundreds of degrees of freedom. Secondly, updates in the CV space are non-local thanks to the generative model, leading to a fast exploration regardless of free energy barriers.

Special requests

Author: GABRIÉ, Marylou**Presenter:** GABRIÉ, Marylou**Session Classification:** Talks

Contribution ID: 29

Type: **not specified**

Machine-Learned Density of States in Multicanonical Simulations

Monday 1 December 2025 14:00 (40 minutes)

Since the density of states (DOS) is the foundation for our capacity to compute thermodynamic characteristics, sample complex energy landscapes, and describe rare-event behaviour, accurately calculating the DOS is a crucial challenge in many fields of computational physics. For applications like neutron spectrum analysis, surrogate modelling of reactor behaviour, and uncertainty quantification in research reactor simulations, accurate DOS estimation is becoming increasingly crucial in nuclear science. Nevertheless, DOS reconstruction is computationally costly and possibly imprecise since conventional Monte Carlo techniques frequently fail to sufficiently sample low-probability energy regions.

To get over these restrictions and enable effective, high-fidelity DOS estimation, we introduce in this work a hybrid multicanonical (MUCA) Monte Carlo–machine learning (ML) system. To create energy histograms with improved coverage of uncommon or otherwise challenging-to-sample areas of the energy domain, the procedure makes use of MUCA sampling. A neural surrogate model that learns a smooth, continuous, and differentiable approximation of the DOS is subsequently trained using these enhanced datasets. The ML-based DOS representation is incredibly quick to assess after training and may be applied to several reweighting jobs without the need for more costly sampling.

We apply the approach to simpler neutron-energy-based models inspired by situations found in research reactor facilities to demonstrate its possibilities. The findings show that while significantly lowering the quantity of MUCA sampling needed, the ML assisted DOS estimator effectively replicates the qualitative characteristics and important structures of the genuine DOS. Additionally, the learnt DOS surrogate makes it possible to evaluate reweighted observables quickly and adaptably, which opens the door to effective parametric investigations and inverse analyses.

All things considered, this hybrid MUCA–ML approach offers a computationally effective basis for combining cutting-edge sampling techniques with contemporary learning methods in reactor simulation. The method has a wide range of potential applications in low-power, training-oriented research reactors and related nuclear systems, including enhancing spectral analysis workflows, speeding up surrogate generation, and assisting with uncertainty quantification and inverse problem-solving

Special requests

Author: APPIAH, KWAME (GHANA ATOMIC ENERGY COMMISSION)

Presenter: APPIAH, KWAME (GHANA ATOMIC ENERGY COMMISSION)

Session Classification: Talks

Contribution ID: **30**

Type: **not specified**

Director's Welcome

Monday 1 December 2025 09:00 (20 minutes)

Opening remarks from ECT* Director Ubirajara van Kolck.

Session Classification: Talks

Contribution ID: **31**

Type: **not specified**

Introduction

Monday 1 December 2025 09:20 (20 minutes)

Introductory remarks and overview of the topics of the workshop.

Special requests

Presenter: KANWAR, Gurtej (University of Edinburgh)

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Crafting Analytic Normalizing Flows

Thursday 4 December 2025 09:40 (40 minutes)

A key challenge in designing discrete normalizing flows is to find expressive parametrized transformations that remain invertible and with tractable Jacobian determinant. Existing approaches face trade-offs: affine transformations are simple but limited, while splines are expressive but piecewise-continuous and bounded. We introduce a family of analytic bijections that are smooth, globally defined, and analytically invertible, bridging the gap between simple and piecewise methods. Besides applying these bijections in coupling flows, we explore novel architectures including interpretable “network free” approaches.

Special requests

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Session Classification: Talks