"Beyond-Metropolis" Markov chains: From the foundations to applications in soft-matter statistical physics, quantum computation, and data science.

Projet de thèse soumis à l'Ecole doctorale EDPIF

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Note: The PhD candidate must either provide his/her own grant or apply for funding through the EDPIF doctoral school

Summary:

The Markov-chain Monte Carlo method is an outstanding computational tool in science [1]. Since its beginning, it has relied on the detailed-balance condition and the Metropolis algorithm to solve general computational problems under the conditions of thermodynamic equilibrium with zero probability flows. Nevertheless, the Metropolis algorithm is slow to reach equilibrium, as the detailed balance generically induces diffusive dynamics.

In recent years, the Monte Carlo framework has been generalized by our research group into irreversible ("Beyond Metropolis") Markov-chain algorithms (notably the event-chain algorithm) that violate detailed balance yet satisfy global balance [2, 3]. Equilibrium is reached as a steady state with non-vanishing probability flows. The famous Metropolis acceptance criterion based on the change in the energy is replaced by a consensus rule. Our research group has since 2015 validated the new paradigm in concrete applications and has in particular demonstrated that the modified Monte Carlo

dynamics is fast and that it converges to the thermodynamic equilibrium notwithstanding the finite probability flows. Results obtained rely on extensive numerical calculations [4, 5, 6], but also on mathematical proofs [7].

Important physical results were obtained for general two-dimensional particle systems [8, 9]. Furthermore, we showed for continuous spin systems that the Beyond-Metropolis algorithm reduces the dynamical critical exponent which quantifies the equilibration process. This indicates that the gain in algorithmic speed can become infinite for large system size. Applications in particle systems have also been very successful [10], allowing to treat even the case of long-range interactions[10, 11]. A major development effort for a Python package using Beyond-Metropolis simulations for soft-matter systems is under way.

The goal of the PhD thesis project is to develop the foundations and the applications of the Beyond Metropolis framework in physics and the neighboring sciences. The project will be developed along (a subset of) the following directions:

- Work on the foundations of the Beyond-Metropolis framework will address algorithmic challenges: How to overcome, categorize, and improve the factorization condition of the system potential and the restriction to infinitesimal moves? How to allow for extended or composite particles (or spins) with internal degrees of freedom? How to establish more mathematical proofs of mixing times? How to evolve the event-chain algorithm? How to understand its recent extensions in quantum field theory [12]? How to extend the recent proofs of mixing times into rigorous statements on the physical phases?

- Work on physical applications will consist, on the one hand in the development of our "JellyFysh" simulation package (written in object-oriented Python3) and on the other hand in its applications, following recent work [11], to short-ranged interacting polymers and solvated peptides in water, among others.

- Work on the extensions will concentrate on the application of the generalized Metropolis algorithm and its close relative, the heat bath algorithm (or Gibbs sampler) in the field of quantum computing. In addition, Markov-chain Monte Carlo methods are also of great importance in the field of data science and machine learning. The use of the Beyond-Metropolis approach for data science will thus also be investigated.

The candidate for this PhD project will be a theoretical physicist with excellent mastery of classical and quantum statistical mechanics, experience with applied mathematics and command of computational physics, with a firm grip on programming in Python (or a willingness to learn).

References

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