Long time simulations of stochastic interacting particle systems

Mireille Bossy^{*1} and Lukasz Szpruch^{†2}

¹INRIA Sophia Antipolis ²University of Edinburgh

Systems of interacting diffusions also called stochastic interacting particle systems (SIPS) and they corresponding Mean-Filed limits have been intensively studied since McKean [4]. These interacting diffusions pave a way to probabilistic representations for many important nonlinear or/and nonlocal PDEs, but provide a great challenge for Monte Carlo simulations. The non-linear dependence of the approximation bias due to the approximation of the dynamics and the statistical error due to the approximation of the measure renders classical variance reduction techniques not directly applicable and consequently simulations of SIPS prohibitive. The high computational cost is even more pronounced when the aim is to simulate SIPS over a long-time horizon. The interest in the long-time simulations arises due to study of the equilibrium/invariant measures for associated McKean-Vlasov SDEs [1]. In this project, we will look at two particular examples of such situations

- Models coming from physics, where the goal is to better understand complex dynamics at the equilibrium
- The effectiveness of Mckean-Vlasov-type dynamics to sample from given probability measure π

Applications to Statistical sampling Diffusion processes provide at the core of many algorithms used in statistics to sample with so-called intractable distributions. These algorithms are often based on some variant of Langevin stochastic dynamics [2]. Given a probability measure π (possibly known up to a normalising constant), the key idea is to construct a diffusion process which admits π as its invariant measure. Then one can run long-time simulations of that diffusion to obtain samples (with some bias) from π . It turns out that by using the ensemble of particles to tune the Langevin dynamics "on the fly" one can significantly improve the efficiency of the method (particularly in the case π is multimodal). This has been recently investigated in [3] by performing numerical experiments. This "on the fly" tuning leads to interactions and in the limit to McKean-Vlasov SDEs.

Applications to Physics Turbulent flow modeling by means of Mckean-Vlasov approaches (so-called Mean Field/PDF stochastic approaches in such domain) is a very active research area, in particular in the domain of Polydispersed turbulent two-phase flows that can be found in numerous environmental and industrial processes (see e.g. [5]). Those approaches couple fluid-particle modeling for turbulence with the description of the motion of solid-particles carried by the flow.

A state of art on numerical methods proposed in such Mean Field/PDF approach can be found in [6], as well as the description of the computational challenges involved by such models. Among them, a long time simulation problem arises through a time re-scaling of the equations that balancing the modeling approach from a kinetic description for solid-particles to a Brownian dynamics approach for the solid phase. Typically, an admissible time-discretization scheme must stay asymptotically stable with respect to the re-scaling parameter.

^{*}mireille.bossy@inria.fr

[†]l.szpruch@ed.ac.uk

Goal of the project

- Construct new Particle representations for McKean-Vlasov SDEs (MVSDEs) with better computational properties
- Develop Multilevel Monte Carlo strategies in the context of MVSDEs on infinite time horizon
- Test various smoothing approaches to singular interaction kernels, involved in applications to physics.
- Investigate different regime parameters such scaling, level of noise, localise interactions

References

- François Bolley, Arnaud Guillin, and Cédric Villani. Quantitative concentration inequalities for empirical measures on non-compact spaces. *Probability Theory and Related Fields*, 137(3-4):541–593, 2007.
- [2] Tony Lelièvre, Gabriel Stoltz, and Mathias Rousset. *Free energy computations: A mathematical perspective*. World Scientific, 2010.
- [3] Charles Matthews, Jonathan Weare, and Benedict Leimkuhler. Ensemble preconditioning for markov chain monte carlo simulation. *arXiv preprint arXiv:1607.03954*, 2016.
- [4] HP McKean Jr. A class of Markov processes associated with nonlinear parabolic equations. Proceedings of the National Academy of Sciences of the United States of America, 56(6):1907, 1966.
- [5] Jean-Pierre Minier. Statistical descriptions of polydisperse turbulent two-phase flows. *Physics Reports*, 665:1 122, 2016. Statistical descriptions of polydisperse turbulent two-phase flows.
- [6] E. Peirano, S. Chibbaro, J. Pozorski, and J.-P. Minier. Mean-field/pdf numerical approach for polydispersed turbulent two-phase flows. *Progress in Energy and Combustion Science*, 32(3):315 – 371, 2006.