# Interacting Particle Systems: Analysis, Control, Learning and Computation
# Poster Session Abstracts
# Wednesday, May 8, 2024

**Emergence of renormalized Hartree-Fock-Bogoliubov and Quantum Boltzmann equations in BECs**

Michael Hott, University of Minnesota - Twin Cities

The derivation of a quantum Boltzmann equation from first principles is a long-standing open problem. There are past conditional results establishing a quartic Quantum Boltzmann equation (QBE). Negative results by Chen-Guo and Chen-Holmer suggest some intricacy when considering weak-coupling limits, as they only obtain a quadratic (=classical) Boltzmann equation in the limit. In the context of Bose-Einstein condensates (BECs), the emergence of Hartree-Fock-Bogoliubov (HFB) equations (think 'buffed up' NLS) has been rigorously established in the mean-field regime from first principles. We will see how to extend previous ideas to describe corrections to the HFB equations by a cubic QBE describing collisions of the BEC with thermal fluctuations, while rigorously controlling the error for times t~(log N)^2. Our results are unconditional.

**Transport based particle methods for the Fokker-Planck-Landau equation**

Vasily Illin, University of Washington

We propose a particle method for numerically solving the Landau equation, inspired by the score-based transport modeling (SBTM) method for the Fokker-Planck equation. This method can preserve some important physical properties of the Landau equation, such as the conservation of mass, momentum, and energy. We prove that matching the gradient of the logarithm of the approximate solution is enough to recover the true solution to the Landau equation with Maxwell molecules. Several numerical experiments in low and moderately high dimensions are performed, with particular emphasis on comparing the proposed method with the traditional particle or blob method.

**Monotonicity for Convergence of Coupled PDEs**

Lauren Conger, California Institute of Technology

We present a notion of $\lambda$-monotonicity for an $n$-species partial differential equation system governed by Wasserstein-2 gradient dynamics. We prove conditions under which monotonicity is sufficient for the existence and uniqueness of a steady state solution, which is a Nash equilibrium for the associated cost functionals. The measures converge at an exponential rate in a joint Wasserstein-2 metric that depends on the monotonicity parameter $\lambda$.

**Function reconstruction using determinantal point processes**

Ayoub Belhadji, Massachusetts Institute of Technology

We study the approximation of a square-integrable function from a finite number of evaluations on a random set of nodes according to a well-chosen distribution. This is particularly relevant when the function is assumed to belong to a reproducing kernel Hilbert space (RKHS). This work proposes to combine several natural finite-dimensional approximations based two possible probability distributions of nodes. These distributions are related to determinantal point processes, and use the kernel of the RKHS to favor RKHS-adapted regularity in the random design. While previous work on determinantal sampling relied on the RKHS norm, we prove mean-square guarantees in norm. We show that determinantal point processes and mixtures thereof can yield fast convergence rates. Our results also shed light on how the rate changes as more smoothness is assumed, a phenomenon known as superconvergence. Besides, determinantal sampling generalizes i.i.d. sampling from the Christoffel function which is standard in the literature. More importantly, determinantal sampling guarantees the so-called instance optimality property for a smaller number of function evaluations than i.i.d. sampling.

**Interacting Particle Systems on Networks: joint inference of the network and the interaction kernel**

Xiong Wang, Johns Hopkins University

Modeling multi-agent systems on networks is a fundamental challenge in a wide variety of disciplines. We jointly infer the weight matrix of the network and the interaction kernel, which determine respectively which agents interact with which others and the rules of such interactions from data consisting of multiple trajectories. The estimator we propose leads naturally to a non-convex optimization problem, and we investigate two approaches for its solution: one is based on the alternating least squares (ALS) algorithm; another is based on a new algorithm named operator regression with alternating least squares (ORALS). Both algorithms are scalable to large ensembles of data trajectories. We establish coercivity conditions guaranteeing identifiability and well-posedness. The ALS algorithm appears statistically efficient and robust even in the small data regime but lacks performance and convergence guarantees. The ORALS estimator is consistent and asymptotically normal under a coercivity condition. We conduct several numerical experiments ranging from Kuramoto particle systems on networks to opinion dynamics in leader-follower models.

**Tensor train based sampling algorithms for approximating regularized Wasserstein proximal operators**

Fuqun Han, University of California, Los Angeles

In this poster, I will present a tensor train based algorithm designed for sampling from a target distribution by approximating the probability density evolution of overdamped Langevin dynamics. The algorithm leverages the regularized Wasserstein proximal operator, which has a simple kernel integration formulation. The integration is evaluated through the assistance of tensor train approximation.

**Sampling in Unit Time with Kernel Fisher-Rao Flow**

Aimee Maurais, Massachusetts Institute of Technology

We introduce a new mean-field ODE and corresponding interacting particle systems (IPS) for sampling from an unnormalized target density. The IPS are gradient-free, available in closed form, and only require the ability to sample from a reference density and compute the (unnormalized) target-to-reference density ratio. The mean-field ODE is obtained by solving a Poisson equation for a velocity field that transports samples along the geometric mixture of the two densities, which is the path of a particular Fisher-Rao gradient flow. We employ a RKHS ansatz for the velocity field, which makes the Poisson equation tractable and enables discretization of the resulting mean-field ODE over finite samples. The mean-field ODE can be additionally be derived from a discrete-time perspective as the limit of successive linearizations of the Monge-Ampere equations within a framework known as sample-driven optimal transport. We introduce a stochastic variant of our approach and demonstrate empirically that our IPS can produce high-quality samples from varied target distributions, outperforming comparable gradient-free particle systems and competitive with gradient-based alternatives.

**Dynamics and Learning for Stochastic Interacting particle systems**

Uresha Dias, Clarkson University

Interacting particle systems, also known as agent-based models, are utilized to study a wide range of physical phenomena across multiple scales; examples include the collective motion of bacteria, the flocking of birds and other animal species, and the coordination of mobile networks. Most such systems exhibit a form of emergence: local interactions which lead to large-scale coordination. A fundamental scientific question is thus discovering local interaction laws which lead to observed behavior. Furthermore, it is well known that in many systems, inter-agent communication is non-deterministic, but instead is influenced by varying degrees of noise. We apply a novel non-parametric statistical learning approach to infer the interaction kernel of agent-based models and assess the ability to learn dynamics, with and without specific emphasis on the learning efficiency as a function of the noise present. We present current results for the deterministic case, applied to models of opinion dynamics and the Lennard-Jones potential, the latter of which is utilized to describe the formation of crystal-like structures. Extensions to stochastic systems are also discussed, with future work being developed for both first- and second-order dynamical systems in the presence of state-dependent noise.

**Brownian dynamics of rigid microspheres in a Stokes fluid**
Irene Erazo, Tulane University

This study investigates the dynamic behavior of small spherical particles subjected to externally applied random forces while immersed in a viscous fluid. Our computational approach uses a regularized Stokeslet formulation. In contrast to the stochastic immersed boundary method, which averages fluctuating random forces within the particle location, here, these forces are in the surrounding fluid, external to the particle surfaces. We assume the particles are spheres with rigid rotations and translations due to the applied transient forces. Moreover, the spheres interact through the fluid, and their trajectories and relative motion are investigated.

**Parametrized Wasserstein Hamiltonian flow**
Shu Liu, UCLA

In this work, we propose a numerical method to compute the Wasserstein Hamiltonian flow (WHF), which is a Hamiltonian system on the probability density manifold. Many well-known PDE systems can be reformulated as WHFs. We use parameterized functions as push-forward maps to characterize the solution of WHF, and convert the PDE to a finite-dimensional ODE system, which is a Hamiltonian system in the phase space of the parameter manifold. We establish theoretical error bounds for the continuous time approximation in Wasserstein metric. For the numerical implementation, neural networks are used as push-forward maps. We design an effective symplectic scheme to solve the derived Hamiltonian ODE system so that the method preserves desirable quantities such as Hamiltonian. The computation is done by a fully deterministic symplectic integrator without any neural network training. The proposed algorithm is a sampling-based approach that scales well to higher dimensional problems. In addition, the method also provides an alternative connection between the Lagrangian and Eulerian perspectives of the original WHF through the parameterized ODE dynamics.

**A deep learning algorithm for computing mean field control problems via forward-backward score dynamics**
Mo Zhou, UCLA

We propose a deep learning approach to compute mean field control problems with individual noises. The problem consists of the Fokker-Planck (FP) equation and the Hamilton-Jacobi-Bellman (HJB) equation. Using the differential of the entropy, namely the score function, we first formulate the deterministic forwardbackward characteristics for the mean field control system, which is different from the classical forward-backward stochastic differential equations (FBSDEs). We further apply the neural network approximation to fit the proposed deterministic characteristic lines. Numerical examples, including the control problem with entropy potential energy, the linear quadratic regulator, and the systemic risks, demonstrate the effectiveness of the proposed method.

**FedCBO: Reaching Group Consensus in Clustered Federated Learning and Robustness to Backdoor Adversarial Attacks**

Sixu Li, University of Wisconsin-Madison

Federated learning is an important framework in modern machine learning that seeks to integrate the training of learning models from multiple users, each user with their own local data set, in a way that is sensitive to the users' data privacy and to communication cost constraints. In clustered federated learning, one assumes an additional unknown group structure among users, and the goal is to train models that are useful for each group, rather than training a single global model for all users. We propose a novel solution to the problem of clustered federated learning that is inspired by ideas in consensus-based optimization (CBO). Our new CBO-type method is based on a system of interacting particles that is oblivious to group memberships. Our algorithm is accompanied by theoretical justification that is illustrated by real data experiments. Motivated from an additional point of concern in federated learning: the vulnerability of federated learning protocols to "backdoor" adversarial attacks, we further introduce a modified, improved particle system with enhanced robustness properties that, at an abstract level, can be interpreted as a bi-level optimization algorithm based on interacting particle dynamics. The poster will surve as a supplement, more focusing on numerical experiments, to the talk given by Nicolás García Trillos on the same topic. The poster is based on the joint works with José A. Carrillo, Nicolás García Trillos and Yuhua Zhu; as well as Aditya Kumar Akash, Nicolás García Trillos, Konstantin Riedl, Deepansha Singh and Yuhua Zhu.

**Dynamics and Learning for Stochastic Interacting particle systems**

Nipuni Senani de Silva Rammini, Clarkson University

Interacting particle systems, also known as agent-based models, are utilized to study a wide range of physical phenomena across multiple scales; examples include the collective motion of bacteria, the flocking of birds and other animal species, and the coordination of mobile networks. Most such systems exhibit a form of emergence: local interactions which lead to large-scale coordination. A fundamental scientific question is thus discovering local interaction laws which lead to observed behavior. Furthermore, it is well known that in many systems, inter-agent communication is non-deterministic, but instead is influenced by varying degrees of noise. We apply a novel non-parametric statistical learning approach to infer the interaction kernel of agent-based models and assess the ability to learn dynamics, with and without specific emphasis on the learning efficiency as a function of the noise present. We present current results for the deterministic case, applied to models of opinion dynamics and the Lennard-Jones potential, the latter of which is utilized to describe the formation of crystal-like structures. Extensions to stochastic systems are also discussed, with future work being developed for both first- and second-order dynamical systems in the presence of state-dependent noise.

**Learning Interaction Variables and Kernels from Observations of Agent-Based Systems**
Ming Zhong, Illinois Institute of Technology

Dynamical systems across many disciplines are modeled as interacting particles or agents, with interaction rules that depend on a very small number of variables (e.g. pairwise distances, pairwise differences of phases, etc...), functions of the state of pairs of agents. Yet, these interaction rules can generate self-organized dynamics, with complex emergent behaviors (clustering, flocking, swarming, etc.). We propose a learning technique that, given observations of states and velocities along trajectories of the agents, yields both the variables upon which the interaction kernel depends and the interaction kernel itself, in a nonparametric fashion. This yields an effective dimension reduction which avoids the curse of dimensionality from the high-dimensional observation data (states and velocities of all the agents). We demonstrate the learning capability of our method to a variety of first-order interacting systems.

**Supervised Learning for Kinetic Consensus Control**
Sara Bicego, Imperial College London

Modeling and control of agent-based models is twice cursed by the dimensionality of the problem, as both the number of agents and their state space dimension can be large. Even though the computational barrier posed by a large ensemble of agents can be overcome through a mean field formulation of the control problem, the feasibility of its solution is generally guaranteed only for agents operating in low-dimensional spaces. To circumvent the difficulty posed by the high dimensionality of the state space a kinetic model is proposed, requiring the sampling of high-dimensional, two-agent sub-problems, to evolve the agents' density using a Boltzmann type equation. Such density evolution requires a high-frequency sampling of two-agent optimal control problems, which is efficiently approximated by means of deep neural networks and supervised learning, enabling the fast simulation of high-dimensional, large-scale ensembles of controlled particles. Numerical experiments demonstrate the effectiveness of the proposed approach in the control of consensus and attraction-repulsion dynamics.