Scientific Computing and Large Data (SCLA)

Dec 16 - Dec 22, 2023

UNIVERSITY OF
South Carolina

Contents

About

This workshop belongs to U of SC and UCLA traditional holiday research breakthrough events. The participants will discuss several interested topics in kernels, PDD dynamics, and sampling optimizations.

Organizing committee

Wuchen Li	University of South Carolina
Siming He	University of South Carolina
Haonan Zhang	University of South Carolina

Timetable

Saturday, Dec 16

9:00–9:50	Lincoln Lu, USC
10:00–11:00	Coffee break
11:00–11:50	Stanley Osher, UCLA
12:00–13:00	Lunch
13:00–15:00	Free discussion
15:00–15:30	Coffee break
15:30–17:00	Free discussion

Sunday, Dec 17

9:00–9:50	Qi Feng, FSU
10:00–11:00	Coffee break
11:00–11:50	Yuan Gao, Purdue
12:00–13:00	Lunch
13:00–15:00	Free discussion
15:00–15:30	Coffee break
15:30–17:00	Free discussion

Monday, Dec 18

9:00–9:50	Yiwei Wang, UC Riverside
10:00–11:00	Coffee break
11:00-11:10	Welcome lecture from Jeff Twiss, Associate Dean
11:10–12:00	Guosheng Fu, Notre Dame
12:00–14:00	Group photo and Lunch
14:00–14:50	Peter Binev, USC

15:00–15:30	Coffee break
15:30–17:00	Free discussion

Tuesday, Dec 19

9:00–9:50	Shu Liu, UCLA
10:00–11:00	Coffee break
11:00–11:50	Mo Zhou, UCLA
12:00–13:00	Lunch
13:00–13:50	Free discussion
14:00–15:00	Bohan Zhou, UCSB
15:00–15:30	Coffee break
15:30–16:30	Hangjie Ji, NC state university

Wednesday, Dec 20

9:00–9:50	Jiajie Zhu, WIAS Berlin
10:00–11:00	Coffee break
11:00–11:50	Xianjin Yang, Caltech
12:00–14:00	Lunch
14:00–15:00	Yifan Chen, NYU
15:00–15:30	Coffee break
15:30–17:00	Free discussion

Thursday, Dec 21

9:00–9:50	Jiaqi Leng, University of Maryland
10:00–11:00	Coffee break
11:00–11:50	Xinzhe Zuo, UCLA
12:00–13:00	Lunch

13:00–15:00	Free discussion
15:00–15:30	Coffee break
15:30–17:00	Free discussion

Friday, Dec 22

9:00–9:50	Report
10:00–11:00	Coffee break
11:00–11:50	Report
12:00–13:00	Lunch
13:00–15:00	Free discussion
15:00–15:30	Coffee break
15:30–17:00	Free discussion

List of Abstracts – Talks

Design of gradient flows for sampling probability distributions

Yifan Chen NYU

Sampling a target distribution with an unknown normalization constant is a fundamental problem in computational science and engineering. Often, dynamical systems of probability densities are constructed to address this task, including MCMC and sequential Monte Carlo. Recently, gradient flows in the space of probability measures have been increasingly popular to generate this dynamical system. In this talk, we will discuss several rudimentary questions of this general methodology for sampling probability distributions. Any instantiation of a gradient flow for sampling needs an energy functional and a metric to determine the flow, as well as numerical approximations of the flow to derive algorithms. We first show how KL divergence is a special and unique energy functional that can facilitate the ease of numerical implementation of the flow. We then explain how the Fisher-Rao metric is an exceptional choice that leads to superior fast convergence of the flow. Finally, we discuss numerical approximations based on interacting particles, Gaussians, and mixtures to derive implementable algorithms for sampling.

Variational Ricci curvature Langevin dynamics: entropy dissipation and its inverse problem

Qi Feng Florida State University

I will first talk about general entropy dissipation for stochastic differential equations. Based on the theoretical guarantees, we design a class of variable coefficient Langevin Markov-Chain-Monte-Carlo (MCMC) methods for sampling non-log-concave target distributions. The algorithm is based on optimization methods for searching “optimal" preconditioners for Langevin Monte-Carlo methods. It solves variational inequalities involving modified Ricci curvatures of target distributions. Under some assumptions and dimension reduction techniques, we can compute this inverse problem independent of dimension. Using its solution, we formulate a class of variable coefficient preconditioners for regular Langevin dynamics, with an exponential convergence guarantee towards the target distribution. Numerical examples with 1D and 2D non-convex functions (non-log-concave target distributions) demonstrate the effectiveness of the proposed methods.

Finite elements meet optimal transport on a Schrodinger bridge

Guosheng Fu University of Notre Dame

We first give a brief introduction of the Monge-Kantorovich optimal transport problem and the closely related Schrodinger bridge problem. The problems can be casted into a (fluid) dynamic formulation through Benamou and Brenier’s celebrated work in 2000. It is a linear (PDE) constrained (convex) optimization problem. We show how finite element methods can be naturally used to discretize this optimization problem, which leads to a discrete saddle point optimization problem. Then a first-order optimization solver, namely, preconditioned Primal-Dual Hybrid Gradient, is used to solve this optimization problem. Numerical results are presented to illustrate the performance of our approach.

Coarsening of thin films with weak condensation

Hangjie Ji NC state university

A lubrication model can be used to describe the dynamics of a weakly volatile viscous fluid layer on a hydrophobic substrate. Thin layers of the fluid are unstable to perturbations and break up into slowly evolving interacting droplets. In this talk, we will present a reduced-order dynamical system derived from the lubrication model based on the nearest-neighbour droplet interactions in the weak condensation limit. Dynamics for periodic arrays of identical drops and pairwise droplet interactions are investigated which provide insights to the coarsening dynamics of a large droplet system. Weak condensation is shown to be a singular perturbation, fundamentally changing the long-time coarsening dynamics for the droplets and the overall mass of the fluid in two additional regimes of long-time dynamics. This is joint work with Thomas Witelski.

Mean field games on continuous and discrete state with applications to rare events and fluid control

Yuan Gao Purdue University

This talk focuses on the Hamilton-Jacobi method for (stochastic) dynamic systems arising from mean-field optimal control problems. We will derive the Hamilton-Jacobi equation (coupled with the Fokker-Planck forward equation) for the mean-field control problem on both continuous and discrete state space. Particularly, for the discrete state space, we introduce various mean-field control formulations: one is suggested by the discrete Wasserstein metric and another one is suggested by the large deviation rate function for jump processes on discrete state space. Some variational properties with applications in rare events and fluid control will be discussed.

On Solving PDEs with Incomplete Information

Peter Binev University of South Carolina

We consider the problem of numerically approximating the solutions to a PDE when there is insufficient information to determine a unique solution. Our main example is the Poisson boundary value problem, when the boundary data is unknown and instead one observes finitely many linear measurements of the solution described by some linear functionals. We view this setting as an optimal recovery problem and develop theory and numerical algorithms for its solution. The main vehicle employed is the derivation and approximation of the Riesz representers of these functionals with respect to relevant Hilbert spaces of harmonic functions. This is a joint research with Andrea Bonito, Albert Cohen, Wolfgang Dahmen, Ronald DeVore, and Guergana Petrova. A preprint is available at arXiv:2301.05540.

A first-order computational algorithm for reaction-diffusion type equations via primal-dual hybrid gradient method

Shu Liu UCLA

We propose an easy-to-implement iterative method for resolving the implicit (or semi-implicit) schemes arising in solving reaction-diffusion (RD) type equations. In our treatment, we formulate the nonlinear time implicit scheme on the space-time domain as a min-max saddle point problem and then apply the primal-dual hybrid gradient (PDHG) method. Suitable precondition matrices are applied to accelerate the convergence of our algorithm under different circumstances. Furthermore, we provide conditions that guarantee the convergence of our method for various types of RD-type equations. We also discuss how the hyperparameters are chosen in order to achieve efficient performance. Several numerical examples as well as comparisons with commonly used numerical methods will also be demonstrated to verify the effectiveness and the accuracy of our method.

Ricci Curvature of Graphs with applications

Lincoln Lu USC

In 2007, Ollivier introduced a notation of Ricci curvature in metric space equipped with a measure or a random walk. In 2011, Lin, Lu, and Yau gave a modified definition of Ollivier-type Ricci curvature on graphs. In this talk, we will study the properties of the Ricci curvature of general graphs, Cartesian product of graphs, random graphs, and some special class of graphs. We will also give some applications. (Joint work with S. T. Yau, Yong Lin, Zhiyu Wang, and others.)

In-Context Operator Learning with Data Prompts for Differential Equation Problems

Stanley Osher UCLA

This talk introduces a new neural-network-based approach, namely In-Context Operator Networks (ICON), to simultaneously learn operators from the prompted data and apply it to new questions during the inference stage, without any weight update. Existing methods are limited to using a neural network to approximate a specific equation solution or a specific operator, requiring retraining when switching to a new problem with different equations. By training a single neural network as an operator learner, we can not only get rid of retraining (even fine-tuning) the neural network for new problems, but also leverage the commonalities shared across operators so that only a few demos in the prompt are needed when learning a new operator. Our numerical results show the neural network's capability as a few-shot operator learner for a diversified type of differential equation problems, including forward and inverse problems of ordinary differential equations (ODEs), partial differential equations (PDEs), and mean-field control (MFC) problems, and also show that it can generalize its learning capability to operators beyond the training distribution.

Energetic variational discretizations of complex fluid models

Yiwei Wang UC Riverside

Motivated by non-equilibrium thermodynamics, the framework of the energetic variational approach (EnVarA) provides a paradigm for constructing thermodynamically consistent variational models for various complex fluids in physics and biology. In this talk, we will present a numerical framework for developing structure-preserving variational discretizations for these models based on their energetic variational forms. The numerical approach begins with the energy-dissipation law, which describes all the physics and assumptions within each system. It can combine different types of spatial discretizations, such as Eulerian, Lagrangian, particle, and neural network-based discretizations. The resulting semi-discrete equation inherits the variational structures from the continuous energy-dissipation law. The numerical procedure ensures that the developed scheme is energy-stable and preserves the intrinsic physical constraints, such as mass conservation and the maximum principle. We will discuss several applications of this numerical approach in solving various PDEs, including porous medium, Fokker-Planck, and reaction-diffusion equations. Additionally, we will also show the developed algorithms can be applied to some machine learning problems.

Inferring strategies and environments from observed populations for mean field games by Gaussian processes

Xianjin Yang Caltech

This paper presents a Gaussian Process (GP) framework, a non-parametric technique widely acknowledged for regression and classification tasks, to address inverse problems inherent in mean field games. By leveraging GPs, we aim to meticulously extract agents' strategic actions and the environment's inherent configurations. Our methodology is grounded on incomplete and noisy observations on the population of agents and the setup of the environment, serving as a vital tool in scenarios where the comprehensive dataset is either inaccessible or prohibitively extensive. The findings highlight the potential of the GP method in facilitating a probabilistic insight into agent behaviors and environmental nuances.

Efficient and Exact Multimarginal Optimal Transport with Pairwise Costs

Bohan Zhou UCSB

Optimal transport has profound and wide applications since its introduction in 1781 by Monge. Thanks to the Benamou-Brenier formulation, it provides a meaningful functional in the image science like image and shape registrations. However, exact computation through LP or PDE is in general not practical in large scale, while the popular entropy-regularized method introduces additional diffusion noise, deteriorating shapes and boundaries. Until the recent work [Jacobs and Leger, A Fast Approach to Optimal Transport: the back-and-forth method, Numerische Mathematik, 2020], solving OT in a both accurate and fast fashion finally becomes possible. Multiple marginal optimal transport is a natural extension from OT but has its own interest and is in general more computationally expensive. The entropy method suffers from both diffusion noise and high dimensional computational issues. In this work with Matthew Parno, we extend from two marginals to multiple marginals, on a wide class of cost functions when those marginals have a graph structure. This new method is fast and does not introduce diffusion. As a result, the new proposed method can be used in many fields those require sharp boundaries.

Advancing Stochastic Optimal Control: An Actor-Critic Framework

Mo Zhou UCLA

Solving the stochastic optimal control problem and its associated Hamilton—Jacobi—Bellman (HJB) equation poses significant challenges due to complexity and non-convexity. In this presentation, we introduce an innovative actor-critic approach tailored to address this complexity. Our method involves deriving an explicit derivative for the cost functional and implementing a policy gradient method for the actor (control) update. The necessity of the current control's value function prompts the development of a policy evaluation process for the critic. We present compelling numerical evidence demonstrating the efficacy of our algorithm and provide rigorous proofs of exponential convergence rates for both the actor and the critic under mild assumptions. Furthermore, we establish a convergence rate for the joint actor-critic dynamics within a single time scale, showcasing the robustness and efficiency of our proposed framework.

Robust Learning under Distribution Shift: Kernel Methods and Gradient Flow Force-Balance

Jia-Jie Zhu WIAS Berlin

I will introduce a variational approach to robust learning algorithms that seek learning and optimization solutions under distribution shifts – discrepancy between the training and test distribution. One of the recent theoretical progress for such learning tasks is the adoption of geometries over probability measures, such as using the Wasserstein distance and kernel maximum mean discrepancy. The heart of our approaches is the explicit parametrization of the generalized force, in the dual space, from the gradient flow perspective. I will demonstrate how this can be used for robust machine learning under joint and structured distribution shifts.

List of Participants

Stanley Osher	UCLA
Lincoln Lu	USC
Hong Wang	USC
Peter Binev	USC
Wuchen Li	USC
Siming He	USC
Haonan Zhang	USC
Guosheng Fu	Notre Dame
Hangjie Ji	NC State University
Jiajie Zhu	WIAS Berlin
Qi Feng	FSU
Yiwei Wang	UC Riverside
Xianjin Yang	Caltech
Bohan Zhou	UCSB
Shu Liu	UCLA
Yifan Chen	NYU
Mo Zhou	UCLA
Xinzhe Zuo	UCLA
Jaiqi Leng	University of Maryland

Useful Information

Zoom link: Meeting ID: 420 256 2026.

Talks will be held at Sumwalt 219, 1212 Greene St. Columbia, SC 29208.

Coffee breaks will be offered in Sumwalt 219, 1212 Greene St. Columbia, SC 29208.

Partner Institutions and Sponsors

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