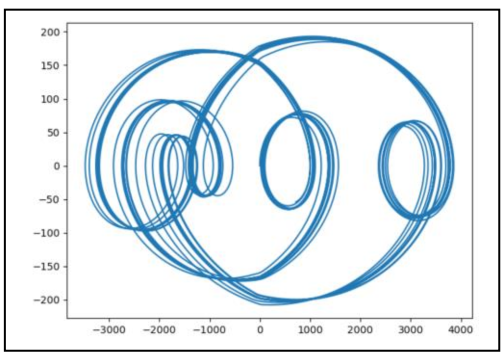
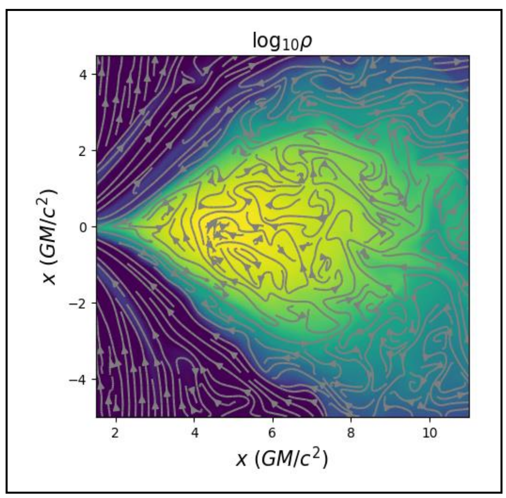
130th Topical Symposium of the
New York State Section of the American Physical Society

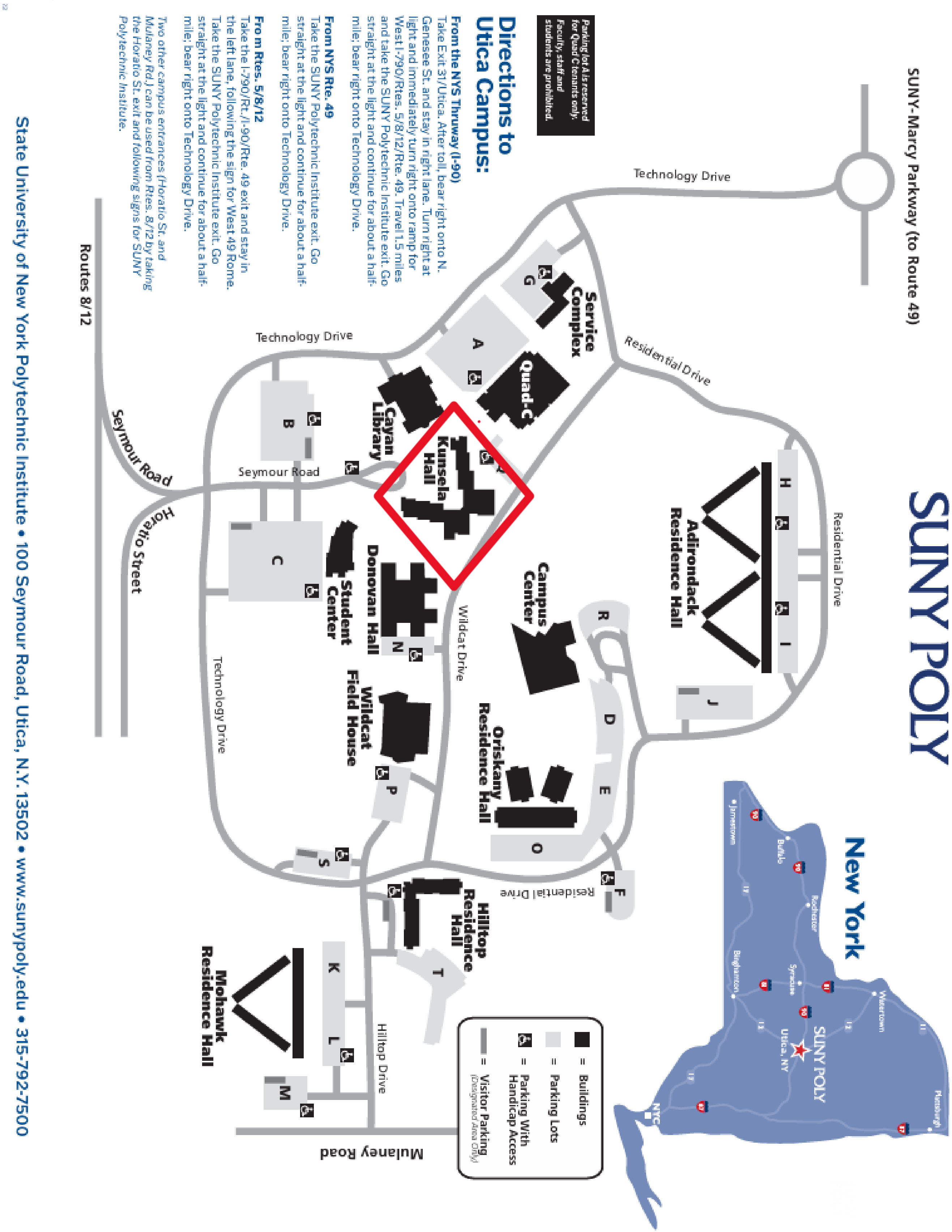
Advances in Computational Physics and the Physics of Computation





Kunsela Hall
SUNY Polytechnic Institute

October 26, 2024



Room A129 MPR, Kunsela Hall, SUNY Polytechnic Institute

Advances in Computational Physics and the Physics of Computation

130th Topical Symposium of the
New York State Section of the American Physical Society
SUNY Polytechnic Institute

nyssaps.org

Schedule of Events

Friday, October 25, 2024

6:30 PM – 7:30 PM Executive Committee Meeting (Room TBD)

Saturday, October 26, 2024

8:30 AM – 9:00 AM Reception/Badge Pickup (Kunsela Hall Foyer)

9:00 AM – 9:15 AM Welcoming Remarks (Kunsela Hall A129 MPR)

9:15 AM – 9:45 AM *Title TBD (Quantum Computation)*
Cameron Cogburn
Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute

9:45 AM – 10:15 AM *Reconstructing Quantum Mechanics from Symplectic and Information Geometry*
Ariel Caticha
Department of Physics, University at Albany

10:15 AM – 10:30 AM Break

10:30 AM – 11:00 AM *MCMC sampling as a metaphor for neural computations*
Ralf Haefner
Department of Brain and Cognitive Science and Department of Physics and Astronomy, University of Rochester

11:00 AM – 11:30 AM *Title TBD (Neural Networks)*
Mirna Skanata
Department of Physics, Syracuse University

11:30 AM – 12:30 PM Lunch (Kunsela Hall Foyer)

12:30 PM – 1:00 PM	*Solving pattern formation and active matter partial differential equations with finite element methods* Alice Quillen Department of Physics and Astronomy, University of Rochester
1:00 PM – 1:30 PM	*Acceleration of materials prediction with machine learning* Alexey Kolmogorov Department of Physics, SUNY Binghamton
1:30 PM – 2:00 PM	*How to model materials properties defined by electron-phonon interactions* Elena Roxana Margine Department of Physics, SUNY Binghamton
2:00 PM – 2:15 PM	**Break**
2:15 PM – 2:45 PM	*Predicting hot electron generation in direct-drive inertial confinement fusion* Chuang Ren Department of Mechanical Engineering and Department of Physics and Astronomy, University of Rochester
2:45 PM – 3:15 PM	*AsterX: a new open-source GPU-accelerated GRMHD code for dynamical spacetimes* Jay Kalinani School of Physics and Astronomy, Rochester Institute of Technology
3:15 PM – 5:00 PM	**Poster Session** (Kunsela Hall Foyer)
5:00 PM – 6:00 PM	**Banquet** (Kunsela Hall Foyer)
6:00 PM – 6:45 PM	**Keynote Presentation** *Lattice Quantum Field Theory: Current Successes and Future Challenges* Simon Catterall Department of Physics, Syracuse University
6:45 PM – 7:00 PM	Award Presentations

Oral Presentations

9:15 AM – 9:45 AM

Title TBD

Cameron Cogburn

Department of Physics, Applied Physics, and Astronomy, RPI

Abstract TBD

9:45 AM – 10:15 AM

Reconstructing Quantum Mechanics from Symplectic and Information Geometry Ariel Caticha

Department of Physics, University at Albany

The symplectic and metric structures inherent in the Hilbert space structure of Quantum Mechanics have been discovered, independently rediscovered, and extensively studied by many authors. Here, rather than postulating those structures as a starting point, we proceed in the opposite direction. Our goal is to "reconstruct" the mathematical formalism of QM from basic considerations of probability theory and information geometry. Our starting point is the recognition that probabilities are central to QM – they are not just a feature that is peculiar to quantum measurements. For simplicity, here we restrict ourselves to the finite dimensional case of a simplex—an *n*-sided die. The important ingredients are two: On one hand the cotangent bundle associated to the simplex has a natural symplectic structure. On the other hand, the cotangent bundle inherits its own natural metric structure from the information geometry of the underlying simplex. We impose a dynamics that preserves (in the sense of vanishing Lie derivatives) both the symplectic structure (a Hamilton flow) and the metric structure (a Killing flow). The resulting Hamilton-Killing flow yields a *realist* ψ*-epistemic model* in which the linearity of the Schrödinger equation, the emergence of a complex structure, Hilbert spaces, and the Born rule, are derived rather than postulated.

A. Caticha, "*The Entropic Dynamics approach to Quantum Mechanics*," Entropy **21**, 943 (2019); arXiv:1908.04693.

A. Caticha, "*Quantum mechanics as Hamilton-Killing flows on a statistical manifold*," Phys. Sci. Forum (2021) **3**, 12; arXiv:2107.08502.

A. Caticha, "*Entropic Dynamics and Quantum Measurement*," Phys. Sci. Forum (2022) **1**, 36; arXiv:2208.02156.

A. Caticha, "*Entropic Physics: Probability, Entropy, and the Foundations of Physics*," online at https://www.arielcaticha.com

Oral Presentations

10:30 AM – 11:00 AM

Title TBD

Ralf Haefner

Department of Brain and Cognitive Science and Department of Physics and Astronomy, University of Rochester

Abstract TBD

11:00 AM – 11:30 AM

MCMC sampling as a metaphor for neural computations

Mirna Skanata

Department of Physics, Syracuse University

Abstract TBD

Oral Presentations

12:30 PM – 1:00 PM

Solving pattern formation and active matter partial differential equations with finite element methods

Alice Quillen

Department of Physics and Astronomy, University of Rochester

Systems described as active matter or pattern forming are confined or influenced by solid, moving or flexible surfaces. By solving partial differential equations on triangular meshes we explore how some pattern formation models are influenced by the proximity and shape of a nearby boundary and the nature of the boundary condition.

1:00 PM – 1:30 PM

Acceleration of materials prediction with machine learning

Alexey Kolmogorov

Department of Physics, SUNY Binghamton

Success of predicting new stable materials depends largely on the scope of the sampled configuration space and the accuracy of the interatomic interaction description. Machine learning interatomic potentials (MLIPs) have emerged as attractive alternatives to traditional interaction-specific potentials designed for large-scale simulations. Being general and flexible approximators, MLIPs can be tuned to describe diverse atomic configurations with near *ab initio* accuracy. I will overview recent advances in the field that have made the construction of reliable MLIPs possible and demonstrate their performance in structure prediction. I will also describe an automated framework for generating representative structure datasets and a stratified scheme for training neural network models for systems with several chemical elements. These approaches implemented in our MAISE package have allowed us to make first predictions of synthesizable compounds.

<u>1:30 PM – 2:00 PM</u>

How to model materials properties defined by electron-phonon interactions

Elena Roxana Margine

Department of Physics, SUNY Binghamton

The coupling between electrons and phonons plays a central role in defining technologically important materials properties, from charge and heat transport to superconductivity and light-driven phase transitions. Recent advances in computational methodology based on maximally-localized Wannier functions have enabled efficient calculations of electron–phonon matrix elements on ultra-dense momentum grids. My group has been leading the effort dedicated to the implementation and consolidation of the anisotropic Wannier-based Migdal-Eliashberg formalism for modeling phonon-mediated superconductors in the open-source EPW package [1]. The methodology allows one to perform highly accurate calculations of the anisotropic temperature-dependent superconducting gap and critical temperature. In this talk, I will present our recent work on the design of conventional high-temperature superconductors synthesizable under ambient conditions.

H. Lee, S. Poncé, K. Bushick, S. Hajinazar, J. Lafuente-Bartolomé, J. Leveillee, C. Lian, J.-M. Lihm, F. Macheda, H. Mori, H. Paudyal, W. H. Sio, S. Tiwari, M. Zacharias, X. Zhang, N. Bonini, E. Kioupakis, E. R. Margine, and F. Giustino, "*Electron-phonon physics from first principles using the EPW code*", NPJ Comput. Mater. **9**, 156 (2023).

<u>2:15 PM – 2:45 PM</u>

Predicting hot electron generation in direct-drive inertial confinement fusion

Chuang Ren

Department of Mechanical Engineering and Department of Physics and Astronomy, University of Rochester

Predicting and controlling hot electron generation from laser-plasma instabilities is a critical challenge in direct-drive inertial confinement fusion (ICF). In this talk we will present progress based on physics-based modeling centered around Particle-in-Cell simulations. We will also present promising preliminary results utilizing generic large language models (LLMs). The ultimate goal is to develop physics-informed ignition-scale LPI packages that can be incorporated into ICF design codes.

Oral Presentations

2:45 PM – 3:15 PM

AsterX: a new open-source GPU-accelerated GRMHD code for dynamical spacetimes

Jay Kalinani

School of Physics and Astronomy, Rochester Institute of Technology

With an increasing demand of extensive parallel computing in numerical simulations addressing various astrophysical problems, codes which can efficiently work on GPUs are the need of the hour. In this talk, I will discuss the salient features of a new open-source general relativistic magnetohydrodynamic (GRMHD) code AsterX, which is built upon CarpetX, a new driver for the Einstein Toolkit. AsterX is based on the flux-conservative Valencia formulation, considering staggered vector potential evolution. It designed to work on GPUs and also takes advantage of the block-structured adaptive mesh refinement provided by CarpetX through the AMReX framework. I will also discuss the various stringent 1D, 2D and 3D GRMHD tests performed with AsterX on the Frontier cluster, and also present scaling results.

Keynote Presentation

6:00 PM – 6:45 PM

Lattice Quantum Field Theory: Current Successes and Future Challenges

Simon Catterall

Department of Physics, Syracuse University

Our understanding of the elementary building blocks of matter and their interactions is encapsulated in the Standard Model of Particle Physics.This is a quantum field theory and the particles observed at experiments such as the Large Hadron Collider at CERN are the elementary excitations of those fields. Certain aspects of the Standard Model can be computed with incredible accuracy using perturbation theory. However the strong interactions of quarks cannot be treated this way and require numerical simulation - this is the field of lattice QCD. I will give an elementary introduction to this theory and highlight some of its main successes in checking aspects of the Standard Model. I will then show how these lattice techniques can be extended to explore the remaining pressing problems in our understanding of the Universe -- what is the physics that keeps the Higgs boson light, why is there more matter than antimatter, what is dark matter and how can we quantize gravity.These are hard problems but I will argue that thinking in terms of quantum field theories in discrete spacetime offers new conceptual and computational tools that can be used to address these questions

Poster Presentations

P1 (UG)

Title

Authors

Affiliations

Abstract

P2 (HS)

Title

Authors

Affiliations

Abstract

P3 (GR)

Title

Authors

Affiliations

Abstract