2022 MATH + X Symposium on Matter under Extreme Conditions in Solar System Giant Planets and Exoplanets, Inverse Problems and Deep Learning

Las Catalinas, Guanacaste, Costa Rica · November 7–9, 2022

funded by

SIMONS FOUNDATION

Abstracts — Monday, November 7

8:30am **David Stevenson** *CalTech*

Why Multicomponent Systems and their Phase Diagrams are Essential for Understanding Planets

Our home planet is layered: An iron-dominated core over a silicate and oxide dominated mantle. This sharp separation is a consequence of Earths low temperature relative to the critical conditions for the intimate mixing of the two end-members. Jupiter is almost(but not quite) in the opposite regime where the two dominant constituents (hydrogen and helium) may be considered well mixed. This strong dichotomy (well mixed and fully separated) is the exception and not the rule among planets and is even somewhat misleading when thinking about our own planets. It is a mistake to imagine that we can understand planets by an obsession with end members (e.g., iron, silicates, hydrogen, water) because the expected temperature and pressure conditions often place us in a regime where the multicomponent aspect becomes essential. After a brief recap concerning H-He (a system that is still imperfectly understood) I will make some observations concerning iron-silicate and its importance of exoplanets (including a denial of the common assumption that these planets should have a core and a mantle). Silicate-hydrogen is also an important binary phase diagram that has major implications for the evolution of so-called superEarths. Hydrogen-water is central to understanding so-called ice giants (e.g., Uranus). More generally, the usual designations that work at low pressure (e.g., polar or non-polar) will break down at high pressure so that components such as methane and water may be less antagonistic at high pressure . The issues before us are computationally difficult, almost invariably involve fluid, not solid, phases (because planets must be hot) and often call out for more experimental guidance, though doubtless there is also a place for simulation. They are not details since they can profoundly affect planetary evolution, presence or absence of a magnetic field, and composition of the atmosphere; in short just about everything you might care to understand or measure.

9:30am **Soledad Villar** *Johns Hopkins University*

Scalars are Universal: Equivariant Machine Learning, Structured Like Classical Physics

There has been enormous progress in the last few years in designing neural networks that respect the fundamental symmetries and coordinate freedoms of physical law. Some of these frameworks make use of irreducible representations, some make use of high-order tensor objects, and some apply symmetry-enforcing constraints. Different physical laws obey different combinations of fundamental symmetries, but a large fraction (possibly all) of classical physics is equivariant to translation, rotation, reflection (parity), boost (relativity), and permutations. Here we show that it is simple to parameterize universally approximating polynomial functions that are equivariant under these symmetries, or under the Euclidean, Lorentz, and Poincaré groups, at any dimensionality d. The key observation is that nonlinear $O(d)$-equivariant (and related-group-equivariant) functions can be universally expressed in terms of a lightweight collection of scalars—scalar products and scalar contractions of the scalar, vector, and tensor inputs. We complement our theory with numerical examples that show that the scalar-based method is simple, efficient, and scalable.

Joint work with David W. Hogg, Kate Storey-Fisher, Weichi Yao and Ben Blum-Smith.

10:45am **Lauri Oksanen** *University of Helsinki*
Inverse Problem for the Wave Equation on Lorentzian Manifolds

The inverse problem for the wave equation asks us to recover the speed of sound given restricted information on solutions to the equation. It models remote sensing using acoustic waves. The problem is well-understood when the speed of sound is independent of time, however, much less is known on the geometric formulation of the problem where the canonical wave equation on a Lorentzian manifold is considered. Inverse problems for several non-linear wave equations, for example, the Einstein equations, can be solved in a very general Lorentzian context, and this gives hope that the corresponding problems for the linear wave equation are solvable as well.

We have developed a method of solving inverse boundary value problems for wave equations on Lorentzian manifolds, and shown that the Lorentzian metric in a fixed conformal class can be recovered under certain curvature bounds. The set of Lorentzian metrics satisfying the curvature bounds is open with respect to smooth enough perturbations of the metric, whereas all previous results on this problem impose conditions on the metric that force it to be real analytic with respect to a suitable time variable. Very recently we were able to weaken the curvature bounds so that perturbations of the Minkowski metric are covered by our theory.

The talk is based on joint work with Spyros Alexakis and Ali Feizmohammadi.

11:30am **Saverio Cambioni** *MIT*
Spotlight: Linking planetary diversity to planet formation processes using machine learning

11:45am **Samory K. Kpotufe** *Columbia University*
From Slow to Fast Rates in Active Learning

In active learning, the learner has the ability to adaptively choose datapoints to label, in contrast with the usual i.i.d. setting where a learner is given a pre-labeled dataset. The hope is to speedup learning, that is, improve performance over what would be achievable with the same amount of i.i.d. labeled data.

Naturally, a main theoretical pursuit over the last decade has been to elucidate the extent to which such speedup is possible. However, the prevalent line of inquiry revealed no such speedup, outside of a few toy examples. Later parametrization of the problem revealed a complex picture: Speedups are guaranteed in some general settings, yet with interesting phase transitions, while no speedup is possible in some seemingly benign settings. These various regimes of speedup are driven by the interplay between label noise, dimension, and feature distributions.

The talk will be devoted to summarizing such findings, and is based on various works with A. Locatelli, A. Carpentier, G. Yuan, and Y. Zhao.

4:00pm **Daniel Thorngren** *Johns Hopkins University*
Giant Exoplanet Population Physics

Extrasolar planet discoveries of the past years have dramatically expanded the set of giant planets available for study, including to extreme conditions not found in the solar system. Unfortunately, the data available for each planet is much more limited and less precise than has been enjoyed for solar system giants. In this talk, I will discuss how we can leverage the large sample size to better understand the interior structure, and evolution of giant exoplanets. In particular, I will review my work on cool giant compositions and hot Jupiter heating and evolution as well as related work by others. I will also discuss how this analysis can synergize with atmospheric observations and the connections with our understanding of planet formation. Finally, Ill outline some future work which could help to push the field forward.

4:45pm **Lorenzo Baldassari** *Rice University*
Spotlight: Inverse source problems for the system of elastic-gravitational equations

5:00pm **Qin Li** *University of Wisconsin-Madison*
Multiscale inverse problem, from Schrödinger to Newton to Boltzmann

Inverse problems are ubiquitous. We probe the media with sources and measure the outputs, to infer the media information. At the scale of quantum, classical, statistical and fluid, we face inverse Schrödinger, inverse Newtons second law, inverse Boltzmann problem, and inverse diffusion respectively. The universe, however, expects a universal mathematical description, as Hilbert proposed in his 6th problem in 1900. In this talk, I would claim that these are equivalent inverse problems presented at different scales, and I will give arguments to justify it.

I would like to invite the audience to brainstorm the scientific and algorithmic consequences. Algorithmically, though the problems are equivalent, the conditionings are drastically different. Are there systematic ways to integrate information across scales? Scientifically in the context of solar systems and matter in the extreme condition, can we translate prohibitive computational tasks to ones that are feasible through the angle of Hilbert's 6th problem?

Abstracts — Tuesday, November 8

8:30am **Stéphane Mallat** *Collège de France*
Generation and Inverse Problems with Deep Wavelet Conditional Models

Optimizing generation and inverse problems amounts to build models of high-dimensional data distributions. Similarly to Wilson renormalisation group, we show that such distributions can be factorised into conditional probabilities of wavelet coefficients across scales, which are typically local and can be log concave. It defines low-dimensional models of complex physical fields such as turbulences, but also of structured images such as faces. It also accelerates score learning in diffusion models of images, by learning simpler and well conditioned conditional probabilities with deep networks. Besides image generation, applications are shown to noise removal and super-resolution recovery.

9:30am **Burkhard Militzer** *University of California, Berkeley*
First-Principles Equation of State Calculations and Application to Jupiter and Saturn

This talk will discuss equation of state calculations and their applications. First, we will describe a first-principles equation of state (FPEOS) database for matter at extreme conditions that we put together by combining results from path integral Monte Carlo and density functional molecular dynamics simulations of eleven elements and ten compounds [1]. For all these materials, pressure and internal energy are provided over a wide density-temperature range from 0.5 to 50 g/cc and from 105 to 109 K. Results from 5000 first-principles simulations were combined. In this talk, we focus on isobars, adiabats and shock Hugoniot curves of different silicates in the regime of L and K shell ionization.

Second, we will discuss the importance of the equation of state of hydrogen-helium mixtures for our understanding of giant planets. We will review the gravity measurements of the Jupiter and Saturn by the Juno and Cassini spacecrafts. Interpreting the Juno measurements has been a challenge because it is difficult to reconcile the unexpectedly small magnitudes of the gravity moments J4 and J6 with conventional interior models that assume a compact core of ice and rock. We show instead that the spacecraft measurements can be matched by assuming that Jupiters cores has been substantially diluted with hydrogen and helium.

[1] B. Militzer, F. Gonzalez-Cataldo, S. Zhang, K. P. Driver, F. Soubiran, "First-principles equation of state database for warm dense matter computation." Phys. Rev. E 103 (2021) 013203. DOI: 10.1103/PhysRevE.103.013203 FPEOS webpage: http://militzer.berkeley.edu/FPEOS

10:45am **Anastasis Kratsios** *McMaster University*
Designing Universal Causal Deep Learning Models: The Case of Infinite-Dimensional Dynamical Systems from Stochastic Analysis

Deep learning (DL) is becoming indispensable to contemporary stochastic analysis; nevertheless, it is still unclear how to design a principled DL framework for approximating infinite-dimensional causal operators. This paper proposes a "geometry-aware" solution to this open problem by introducing a DL model-design framework that takes a suitable infinite-dimensional linear metric spaces as inputs and returns a universal sequential DL models adapted to these linear geometries. Our main result states that the models produced by our framework can uniformly approximate on compact sets and across arbitrarily finite-time horizons Hölder or smooth trace class operators which causally map sequences between given linear metric spaces. Consequentially, we deduce that a single CNO can efficiently approximate the solution operator to a broad range of SDEs, thus allowing us to simultaneously approximate predictions from families of SDE models, which is vital to computational robust finance. We deduce that the CNO can approximate the solution operator to most stochastic filtering problems. Our universal approximation results estimate the complexity of the CNO model in terms of the involved spaces' geometries, the regularity of the causal operator (that is, its smoothness or Hölder regularity and the persistence of its memory on the distant past), and the desired approximation error. Our quantitative analysis shows that a linear increase of the CNO's latent parameter space's dimension, width and a logarithmic increase in its depth imply an exponential increase in the number of time steps for which its approximation remains valid. Moreover, our approximation guarantees are superoptimal compared to the optimal approximation rates for ReLU networks when approximating real-valued maps from a high-dimensional Euclidean space with a causal structure.

11:30am **Haim Grebnev** *University of Washington*
Spotlight: The Non-Abelian X-Ray Transform

11:45am **Carlo Pierleoni** *University of L'Aquila*
Phase Diagram and Optical Properties of Hydrogen Under Extreme Conditions

The knowledge of the equation of state and the physics of high pressure hydrogen, in particular across the molecular dissociation and system metallization, is one of the key information to develop accurate models for the interior of Giant gas planets of the Solar system and for recently discovered exoplanets. We present a survey of the present understanding of the hydrogen phase diagram under high pressure conditions and temperature range covering melting of the crystal and the metallization both in the solid and in the fluid phase. We will highlight the emerging picture from ab-initio Quantum Monte Carlo methods and discuss the comparison with experiments in various conditions.

4:00pm **Roberto Car** *Princeton University*
Machine Learning Based Ab-initio Molecular Dynamics

Computational cost severely limits the range of ab initio molecular dynamics simulations. Machine learning techniques are rapidly changing this state of affairs. Deep neural networks, that learn the interatomic potential energy surface from ab-initio data, make possible simulations with quantum mechanical accuracy at the cost of empirical force fields. These approaches can model not only atomistic dynamics but also the dielectric response properties measured in experiments. I will discuss, in particular, the deep potential method developed at Princeton. In combination with incremental learning techniques, this approach makes possible to construct, with minimal learning cost, reactive potentials that are accurate over a vast range of thermodynamic conditions, such as the pressure and temperature regimes underlying molecular and ionic phases of water. Topics of interest for high pressure physics will be discussed.

5:00am **Hope Jasperson** *Rice University*
Spotlight: Generalized Optimizer for Unsupervised Deep Assignment

5:15pm **Matti Lassas** *University of Helsinki*
Inverse Problems for Graphs and Discrete Spaces

We study the inverse problem of determining a finite weighted graph (X, E) from the source-to-solution map on a vertex subset $B \subset X$ for heat equations on graphs, where the time variable can be either discrete or continuous. We prove that this problem is equivalent to the discrete version of the inverse interior spectral problem, provided that there does not exist a nonzero eigenfunction of the weighted graph Laplacian vanishing identically on B. In particular, we consider inverse problems for discrete-time random walks on finite graphs. We show that under the Two-Points Condition, the graph structure and the transition matrix of the random walk can be uniquely recovered from the distributions of the first passing times on B, or from the observation on B of one realization of the random walk. In addition, we will consider the problem of approximating discrete metric spaces or graphs by smooth manifolds.

Abstracts — Wednesday, November 9

8:30am **Chris Pickard** *University of Cambridge*
Mapping the Complex Chemistry of Dense Matter

First principles methods for the prediction of structures and chemistry at high pressures have delivered a powerful tool for the computational exploration of dense matter. While early studies focused on the exotic properties of relatively simple systems, typically the elements and binary compounds, much of the matter in the Universe is likely to be found in more complex mixtures [1]. At the same time, the promise of discovering materials with extreme properties relies on the ability of screen a wide variety of compounds [2]. I will reflect on why ab initio random structure searching (AIRSS) is particularly suited to these challenges, and the importance of visualising the vast datasets we are now generating [3].

[1] Conway, Lewis J., Chris J. Pickard, and Andreas Hermann. “Rules of formation of H-C-N-O compounds at high pressure and the fates of planetary ices.” Proceedings of the National Academy of Sciences 118, no. 19 (2021).

[2] Shipley, Alice M., Michael J. Hutcheon, Richard J. Needs, and Chris J. Pickard. "High-throughput discovery of high-temperature conventional superconductors." Phys. Rev. B 104, 054501 (2021).

[3] Shires, Ben W.B., and Chris J. Pickard. "Visualising energy landscapes through manifold learning." Phys. Rev. X 11, 041026 (2021).

9:30am **Ivan Dokmanić** *University of Basel*
Learning Graphs, Manifolds and Bundles by Playing Trumpets and Pooling Walks

A low-dimensional manifold is probably the most successful data model after the venerable linear subspace. Popular data visualization tools like tSNE operate under the manifold assumption; patches of natural images are topologically a Klein bottle; invariant manifolds give low-dimensional representations of dynamical systems; key inverse problems like traveltime tomography are equivalent to manifold learning. I will present ongoing research in my group which combines graph theory, complex networks, and differential geometry to build machine learning tools for data on manifolds and graphstheir discrete counterparts. Modeling manifold-supported probability measures with injective flows (which we call Trumpets) gives priors and algorithms for inverse problems. Conditional Trumpets model data on fiber bundles and enable eicient Bayesian inference. Insights from statistical physics and complex networks inspire a state-of-the-art link prediction algorithm which is transmogrified into a tool to learn manifolds under extreme noise. Applications to inference and inverse problems abound.

10:45am **Joonas Ilmavirta** *University of Jyväskylä*
Spectral Rigidity of Radial Planets

I will discuss from the mathematical point of view whether the spectrum of free oscillations uniquely determines the structure of a radial planet. I will cover general formulations, typical tools, and types of theorems. The most recent results of planetary relevance show that under some reasonable conditions a radial velocity profile is uniquely determined by the spectrum in a certain linearized sense.

11:30am **Jinpeng Lu** *University of Helsinki*
Spotlight: Quantitative Unique Continuation for Wave Equations, Seismicity and the Kinematic Inverse Rupture Problem

11:45am **Carlos Fernandez-Granda** *New York University*
Evaluating Unsupervised Denoising Requires Unsupervised Metrics

Denoising is a crucial challenge in imaging applications. In recent years, unsupervised methods based on deep learning have demonstrated impressive performance on natural-image benchmarks. However, no quantitative metrics are available to evaluate these methods in an unsupervised fashion. This is highly problematic for the many real-world applications where ground-truth clean images are not readily available. In this talk we introduce two novel metrics: the unsupervised mean squared error (MSE) and the unsupervised peak signal-to-noise ratio (PSNR), which are computed using only noisy data. We provide a theoretical analysis of these metrics, which shows that they are asymptotically consistent estimators of the supervised MSE and PSNR. Controlled numerical experiments with synthetic noise confirm that they provide accurate approximations in practice. To illustrate their potential impact, we report experiments with real-world data from two imaging modalities: videos in raw format and transmission electron microscopy.

2:00pm **Tristan Guillot** *Observatoire de la Côte dAzur*
Unveiling Jupiters Interior with Juno

Jupiter shaped our Solar System but its internal structure and composition remain mysterious. The Juno spacecraft, in orbit since 2016, has enabled extremely accurate measurements of its gravity and magnetic fields. It has also probed the planets deep atmosphere thanks to its microwave radiometer. I will review the advances that have been possible thanks to these measurements, including the determination of the depth of Jupiters zonal flows, the detection of secular variations of its magnetic field, the presence of compositional gradients in the deep atmosphere. Interior models possible with these constraints indicate that Jupiters envelope is inhomogeneous and that its core is most likely partially diluted. I will show how constraints on its internal structure and composition rest on our knowledge of the behavior of matter at very high pressures and require extensive calculations, to cope both with a vast parameter space and a difficult minimization problem. Measurements of the planet's oscillations, already possible for Saturn, should further improve our knowledge of the planetary interior and composition.

2:45pm **Hieu Huu Nguyen** *University of Basel*
Spotlight: Implicit Neural Representation and Lens Rigidity, Unveiling Planetary Interiors

3:00pm **Michael Puthawala** *Rice University*
Spotlight: Deep Invertible Approximation of Topologically Rich Maps between Manifolds and Uncertainty Quantification

3:15pm **Santiago Segarra** *Rice University*
Principled Simplicial Neural Networks for Trajectory Prediction

We consider the construction of neural network architectures for data on simplicial complexes. In studying maps on the chain complex of a simplicial complex, we define three desirable properties of a simplicial neural network architecture: namely, permutation equivariance, orientation equivariance, and simplicial awareness. The first two properties respectively account for the fact that the node indexing and the simplex orientations are arbitrary. The last property encodes the desirable feature that the output of the neural network depends on the entire simplicial complex and not on a subset of its dimensions. Based on these properties, we propose a simple convolutional architecture, rooted in tools from algebraic topology, for the problem of trajectory prediction, and show that it obeys all three of these properties when an odd, nonlinear activation function is used. We then demonstrate the effectiveness of this architecture in extrapolating trajectories on synthetic and real datasets, with particular emphasis on the gains in generalizability to unseen trajectories.