2023 MATH + X Symposium on Dynamos, Planetary Exploration and General Relativity, Inverse Problems and Machine Learning

Hella, Iceland · May 29 – June 1, 2023

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Abstracts — Monday, May 29

8:30am **Raymond Pierrehumbert** *University of Oxford*

Keynote: Dynamical problems and emergent properties in exoplanet climate

Tide-locked exoplanets, when in near-circular orbits, always present the same face to their host star, the way the Moon always presents the same face to the Earth. This drives dramatic circulations with a dominant wave-1 forcing. I will discuss atmospheric circulation regimes of tide-locked exoplanets, drawing on concepts developed in connection with the Earths tropics. Wave-Mean-Flow interactions and their role in generation of equatorial super-rotation will be discussed, together with intrinsically three-dimensional effects that are not captured by shallow-water dynamics

9:15am **Rafe Mazzeo** *Stanford University*

The analysis of Kimura-type operators

Elliptic operators with simple degeneracies at boundaries appear in many applications. I will describe some work with Epstein, originating in population dynamics, that provides a means to understand many properties of these operators, some of which are suitable for numerical methods. I will also describe other techniques, from microlocal analysis, which provide other insights into these operators.

10:30am **Chirag Modi** *Flatiron Institute*

Reconstructing the initial conditions of the Universe

Over the last decade, cosmologists have turned to developing a novel way of analyzing cosmology survey data with reconstructing the Gaussian initial conditions at the beginning of the Universe, and other latent cosmological fields. This requires solving a challenging high dimensional inverse problem with an expensive, non-linear forward model: a cosmological N-body simulation. In this talk, I will begin by outlining why we are interested in reconstructing these initial conditions of the Universe. I will then present two major technical advances made over the last couple years to make this exercise tractable. First, I will discuss the automatically differentiable N-body solvers that we have developed in ML frameworks. Next, I will touch upon how these simulations can be combined with machine learning tools like recurrent networks and normalizing flows to accelerate Bayesian inference algorithms in high dimensions by learning an optimization path to the maximum-a-posteriori (MAP) estimate or reducing the correlation length for MCMC samples.

11:15am **Michael Bronstein** *University of Oxford*

Physics-inspired learning on graphs

The message-passing paradigm has been the “battle horse” of deep learning on graphs for several years, making graph neural networks a big success in a wide range of applications, from particle physics to protein design. From a theoretical viewpoint, it established the link to the Weisfeiler-Lehman hierarchy, allowing to analyse the expressive power of GNNs. We argue that the very node-and-edge-centric mindset of current graph deep learning schemes may hinder future progress in the field. As an alternative, we propose physics-inspired continuous learning models that open up a new trove of tools from the fields of differential geometry, algebraic topology, and differential equations so far largely unexplored in graph ML.

1:30pm **Philippe Lognonné** *Institut de Physique du Globe de Paris*

Discovering Mars interior structure with SEIS-InSight Data

The SEIS seismometer of the InSight mission operated on Mars from February 2019 to December 2022 and has returned the first collection of seismic data from Planet Mars. More than 1300 seismic events, including $\sim$10 impacts and a large M $\sim$4.7 event have been detected, with several hundred events originating from Cerberus Fossae, a place about 1600 km away from InSight where recent dyke volcanism is found. We first present the experiment, the observation limitations and Mars seismicity, for both marsquakes and impacts. We then present the different techniques which have been used to extract from a single seismic record a set of seismic observables useful for seismic inversion and which include for seismic events first and secondary arrival times, back-azimuth, surface wave dispersion curves (for 3 large events), possible normal modes (for one large event), receiver functions, site effects and compliance (for more crustal and subsurface structure) and even atmospheric infrasound dispersion curves (for several impacts). We then develop how Monte-Carlo approaches have been used, together with a priori geophysical and mineralogical modeling of the core, mantle, crust and near-surface atmospheric boundary layer, in order to interpret these data in terms of Bayesian inference of the interior parameters of Mars, which include core radius, mantle structure, crustal and subsurface structure, and of the first km of the atmosphere.

2:15pm **Stéphane Mallat** *Collège de France*

Multiscale random models of deep neural networks

A major issue is to understand how deep networks avoid the curse of dimensionality to generate and classify complex data. Inspired by the renormalization group in physics, we explain how deep networks can separate phenomena which appear at different scales, and capture scale interactions. Depending upon the underlying physical phenomena, this scale interaction needs to be learned. We show that for large classes of physical processes, such learning is linearized by random projections. It is proved to be equivalent to particular high order moment expansions. Models of deep network learning for image classification are also obtained with cascades of random projections across scales.

3:30pm **Peter Constantin** *Princeton University*

Keynote: Nonlocality in fluids: Electrostatic interactions

I'll describe models of electroconvection and ionic diffusion in fluids. These models include naturally ocurring nonlocal interactions due to the Lorentz force and due to the geometry of the devices. I will give a bit of background and present some of the recent results.

4:30pm **Siddharth Mishra-Sharma** *Massachusetts Institute of Technology*

Solving inverse problems in cosmology with simulation-based inference and generative modeling

The next several years will witness an influx of astrophysical data that will enable us to accurately map out the distribution of matter in the Universe, image billions of stars and galaxies to unprecedented precision, and create the highest-resolution maps of the Milky Way to-date. The complexity of the data and the presence of unknowable systematics pose significant challenges to robustly extracting information about fundamental physics using conventional methods. I will describe how overcoming these challenges will require a qualitative shift in our approach to statistical inference in cosmology and astrophysics, bringing together several recent advances in generative modeling, differentiable probabilistic programming, and simulation-based inference.

5:00pm **Shirley Ho** *Flatiron Institute*

Generative AI for science

With the rapid evolution of generative AI, I will discuss a few application and development of generative AI tools for science.

Abstracts — Tuesday, May 30

8:30am **Nikku Madhusudhan** *University of Cambridge*

Keynote: Habitability in the sub-Neptune regime

Sub-Neptunes, with radii between those of Earth and Neptune, dominate the exoplanet population. In particular, sub-Neptunes orbiting M-dwarfs present a promising avenue for their detection and atmospheric characterisation, including those in the habitable zones of their host stars. Traditionally, notions of planetary habitability have focused on predominantly rocky exoplanets and ocean worlds with terrestrial-like atmospheric compositions. In this talk, I will discuss the possibility of habitable conditions on a subset of temperate sub-Neptunes with water-rich interiors and hydrogen-rich atmospheres, called Hycean worlds. Such planets can be larger and hotter than terrestrial-like habitable planets, significantly expanding the habitable zone, and are substantially more abundant and observable in the solar neighbourhood. We will discuss the theoretical developments underlying this new paradigm and their observational implications.

9:15am **Anna Mazzucato** *Pennsylvania State University*

Shape derivative for an inverse problem in fault monitoring

We consider a model of elastic dislocations in geophysics with applications to fault monitoring, and derive a shape derivative under infinitesimal movements of the fault and infinitesimal changes in the slip along the fault. We then implement an iterative algorithm based on the shape derivative to reconstruct the fault geometry and slip vector from surface displacement measurements.

This is joint work with A. Aspri, E. Beretta and P. Antonietti.

10:30am **Lina Necib** *Massachusetts Institute of Technology*

The genealogy of the Milky Way and the search for the missing dark matter

Galaxies form and grow by merging with other galaxies, making the formation history of a galaxy resemble that of a family tree. Our galaxy, the Milky Way, is no exception, and with recent telescopes like Gaia, we are able to build the Milky Way's family tree. We find that a large galaxy, called Enceladus after the Greek giant son of Gaia, merged with the Milky Way about 10 billion years ago, leaving a large trail of old stars. However, these mergers did not only bring in stars, but also something unseen, the Dark Matter, a hypothesized matter making up 86% of the local universe but is yet to be directly detected. These ethereal Dark Matter particles have different dynamics from the ones born in the Milky Way, affecting Dark Matter searches by creating local dark hurricanes. In this talk, I will show you amazing videos of simulated merging galaxies, and emphasize how these mergers have direct implications on our searches for the mysterious Dark Matter.

11:15am **Gunther Uhlmann** *University of Washington, Hong Kong University of Science and Technology*
Some inverse problems in general relativity

Abstracts — Wednesday, May 31

8:30am **Michael Brenner** *Harvard University*
Keynote: Scientific uses of automatic differentiation

There is much excitement about applications of machine learning to the sciences. Here I'm going to argue that a primary opportunity is not machine learning per se, but instead that the tools underlying the ML revolution yield significant opportunities for scientific discovery. Primary among these tools is automatic differentiation. I will outline a number of different directions we have been undertaking using automatic differentiation and large scale optimization to solve science problems, including developing new algorithms for solving partial differential equations, the design of energy landscapes and kinetic pathways for self assembly, the discovery of unstable solutions controlling fluid dynamical instabilities, the development of models for organismal development, implementing protocols in nonequilibrium statistical mechanics, a priori design of fluid rheology the design of chaotic mixing strategies and so forth. My main point is to highlight opportunities and ways of thinking.

9:15am **Elena Beretta** *New York University Abu Dhabi*
On the detection of cavities in an elastic medium from boundary measurements

Detection of cavities in elastic media from boundary measurements has several applications in seismology, geophysics and nondestructive testing of materials. The related inverse boundary value problems are severely ill-posed, making the reconstruction a challenging issue. In my talk I will first survey some results concerning uniqueness and stability, and then describe some recent results concerning a reconstruction algorithm based on a phase field approach.

10:30am **Richard Teague** *Massachusetts Institute of Technology*
Witnessing the earliest stages of planet formation

We have observed a stunning diversity in the properties of exoplanetary systems which questions our understanding of planet formation. Does this diversity arise from differences in initial conditions? Are there multiple modes of planet formation which preferentially build different types of planets? Or does this diversity stem from the evolution of the newly born planetary system as the natal protoplanetary disk dissipates? Over the last several years we have gained an incredible insight into how planetary systems form and evolve thanks to facilities such as ALMA which allow us to resolve — spatially and spectrally — these planetary nurseries. In this talk I will discuss how our view of the protoplanetary disk has shifted from a smooth, flat 2D disk, to a highly structured and vertically extended disk which hosts complex flows and dynamical features driven by embedded planets. I will provide examples of how these observations, coupled with state-of-the-art numerical simulations, are shining new light on the planet formation process, and how new facilities, such as JWST, are going to allow us to tackle new questions related to our origins.

11:15am **Ivan Dokmanić** *University of Basel*
Trawling for networks in dynamics

Interactions in complex dynamical systems in physics, biology, neuroscience, and Earth science are key to their function. It is usually challenging to determine interactions directly: measuring neuronal connectivity requires painstaking analyses of electron microscopy images, functional brain connectome cannot even be uniquely defined, and we have no idea how to measure stress transfer between faults in geological fault systems. At the same the cornucopia of new sensor measurements makes it extremely attractive to determine interactions from the observed dynamics alone. I will show how graph neural networks can be used to build effective priors for relational inference from dynamics but also how an interaction-centric perspective yields insight into GNNs themselves.

1:30pm **Rose Yu** *University of California San Diego*
Keynote: Physics-guided AI for learning spatiotemporal dynamics

Applications in science often require learning complex dynamics from large-scale spatiotemporal data. While deep learning has shown tremendous success in these domains, it remains a grand challenge to incorporate physical principles in a systematic manner into the design and training of such models. In this talk, I will demonstrate how to principally incorporate physics in AI models to improve sample complexity, prediction accuracy, and physical consistency. I will showcase the applications of these models to challenging problems such as turbulence forecasting in climate science, jet tagging in particle physics, and trajectory prediction for autonomous vehicles.

2:15pm **Matti Lassas** *University of Helsinki*
Mapping properties of neural networks and inverse problems

We will consider mapping properties of neural networks, in particular, injectivity of neural networks and universal approximation property of injective neural networks. In addition, we study approximation of probability measures using neural networks that are compositions of invertible flow networks and injective layers. We also present applications in inverse problems.

The results have been done in collaboration with M.V. de Hoop, I. Dokmanić, P. Pankka and M. Puthawala.

3:30pm **Michael Mahoney** *University of California, Berkeley*
Foundations for scientific machine learning

Delivering on the promise of scientific machine learning will require going beyond using machine learning methods (typically developed for very different industrial applications and implemented in very different computational environments) to developing novel machine learning methods that are well-suited to the needs of science. I will describe several examples of this from recent work: one that uses methods from numerical integration theory to go beyond traditional machine learning training/testing methodology on discrete data to test whether the learned function is meaningfully continuous; another that identifies fundamental limitations with existing "physics informed" approaches; and another provides a framework to incorporate conservation constraints into a generic SciML architecture, seamlessly enforcing physical conservation constraints, maintaining probabilistic uncertainty quantification (UQ), and dealing well with shocks and heteroscedasticities arising with relatively "hard" (e.g., hyperbolic) PDE operators.

4:30pm **Benjamin Weiss** *Massachusetts Institute of Technology*

History of the solar nebula from meteorite paleomagnetism

A key stage in planet formation is the evolution of a gaseous and magnetized solar nebula. However, the intensity of the nebular field, the lifetime of the nebula, and the history of mass transport in the early solar system have been poorly constrained. Here we present analyses of the remanent magnetization in several meteorite groups demonstrating that an approximately Earth-strength ($\sim 50\,\mu$T) nebular magnetic field existed in the inner and outer solar system (~ 1–10 AU) during the first 1–3 My after solar system formation. The nebular field then declined to near-zero ($< 0.1\mu$T) in the $\sim$1–10 AU region by $\sim$4 My after solar system formation, suggesting that the solar nebula field, and likely the nebular gas, had globally dispersed by this time. This sets the timescale for formation of the gas giants and disk-driven planet migration and supports the hypothesis that giant planets form by a two-stage process involving formation of a rock-ice core followed by runaway gas accretion. Our magnetic measurements of volatile-rich carbonaceous meteorites and comet 67P Churyumov-Gerasimenko provide evidence for dynamical mixing of solids over tens of AU and indicate that we may have rock samples from the proto-Kuiper belt. Finally, our recent paleomagnetic studies of refractory inclusions have identified evidence for a $\sim 150\,\mu$T field, the oldest known paleomagnetic record. This provides evidence for transient accretion bursts that likely played a significant role in formation of the sun and the first solar system solids.

5:00pm **Otmar Scherzer** *University of Vienna*

Newton methods for solving linear inverse problems with neural network coders

Neural network functions are considered to be able to describe the desired solution of an inverse problem very efficiently, thus allowing for sparse encoding of the desired reconstruction. In this work we consider the problem of solving linear inverse problems with neural network coders with a Gauss-Newton method. In an abstract setting this problem has been considered for some time, for instance under the name of state space regularization. In this paper, we prove local convergence results for Gauss-Newton methods.

This is a joint work with L. Frischauf, B. Hofmann, Z. Nashed and C. Shi.

Abstracts — Thursday, June 1

8:30am **Josselin Garnier** *École Polytechnique, Paris*

Reduced order model approach for imaging with waves

We consider the inverse problem for the scalar wave equation. Sensors probe the unknown medium to be imaged with a pulse and measure the backscattered waves. The objective is to estimate the velocity map from the array response matrix of the sensors. Under such circumstances, conventional Full Waveform Inversion (FWI) can be carried out by nonlinear least-squares data fitting. It turns out that the FWI misfit function is high-dimensional and non-convex and it has many local minima. A novel approach to FWI based on a data-driven reduced order model (ROM) of the wave equation operator is introduced and it is shown that the minimization of ROM misfit function performs much better.

The talk is based on a joint work with L. Borcea (Univ. Michigan), A. Mamonov (Univ. Houston), J. Zimmerling (Uppsala Univ.)

9:15am **Giovanni Alberti** *University of Genoa*

Machine learning for infinite-dimensional inverse problems

In recent years, machine learning techniques have become very popular to solve inverse problems. Inverse problems are ubiquitous in science and engineering, and appear whenever a physical quantity has to be reconstructed from indirect measurements. Inverse problems are typically ill-posed, meaning that small errors in the measurements may have large effects in the reconstruction. Classically, regularisation is used to overcome ill-posedness, but prior knowledge on the unknown is needed for the choice of regularisation. Machine learning comes into play as a way to make regularisation, and more generally the inversion process, data-driven, thanks to the use of a training set. Many inverse problems are modelled by integral or differential operators and, consequently, are intrinsically infinite-dimensional. In this talk, I will discuss how machine learning can be rigorously used in infinite-dimensional inverse problems, in the context of learning the optimal regulariser or by using generative models in function spaces.

10:30am **Alexei Iantchenko** *Malmö University*

Inverse problems in surface-wave tomography with spectral and resonance data

Semiclassical analysis can be employed to describe surface waves in an elastic half space which is quasi-stratified near its boundary. In the case of an isotropic medium, the surface wave decouples up to principal parts into Love and Rayleigh waves associated to scalar and matrix spectral problems, respectively. Since the mathematical features (such as spectrum, resonances) of these problems can be extracted from the seismograms, we are interested in recovering the Lamé parameters from these data. We generalize spectral methods for Schrödinger operators to the Rayleigh problem, which is essentially not of Schrödinger type; and give comprehensive analysis of the wavenumber resonances, known in seismology as leaking modes.

This is joint work with M.V. de Hoop.

11:15am **Jiequn Han** *Flatiron Institute*

A neural network warm-start approach for inverse scattering problems

Inverse scattering problems play a crucial role in numerous applications across various fields. However, the widely-used optimization formulation is challenging to solve due to the computationally expensive evaluation of the objective function and the problem's highly nonlinear, non-convex, and ill-posed nature. In this talk, we introduce a neural network warm-start approach to effectively tackle these challenges while maintaining high precision. We will discuss the benefits of our approach, its implications, and how it can contribute to enhancing current practices in the field. The underlying philosophy of this method has the potential to be applied to a broader range of scientific challenges in the field of PDEs that demand low computational costs and high accuracy.

11:45pm **Joonas Ilmavirta** *University of Jyväskylä*

Imaging the universe with a gaugeless theory of conformal geometry

The concept of a geodesic on a Lorentzian manifold needs to be redefined to make it invariant under all changes of parameter and all conformal scalings of the metric tensor. Such a redefined concept is useful for the study of cosmological inverse problems based on geometric measurements of light, as they necessarily exhibit a conformal gauge freedom.

This is based on joint work with M.V. de Hoop, H. Hänninen, M. Lassas and T. Saksala.