Workshop

Challenges and Benchmarks for quantitative AI in Complex Fluids and Complex Flows

Centro Ricerche Enrico Fermi

Piazza Viminale 1, Rome, Italy 6-8 JULY 2022

6 JULY

10.30-11.45 - Registration + Welcome Coffee

11.45-11.55 - Welcome - **Luciano Pietronero** President of Centro Ricerche Enrico Fermi

11.55-12.00 - Welcome - **Luca Biferale**, **Michele Buzzicotti** and **Massimo Cencini**

12.00-12.30 - *"There is plenty of room in the middle: Alloys of Scientific Computing and Machine learning"* - **Petros Koumoutsakos**

Over the last thirty years we have experienced more than a billion-fold increase in hardware capabilities and a dizzying pace of acquiring and transmitting massive amounts of data. Artificial Intelligence (AI) has been the beneficiary of these advances and today it is increasingly embedded in technologies that touch every aspect of humanity. It is often advocated that AI can bypass many of the challenges for advancing Computational Science. In this talk I would offer a perspective on forming alloys of AI and simulations for the prediction and control of complex flow systems. I will present novel algorithms for learning the Effective Dynamics (LED) of complex flows and a fusion of multi-agent reinforcement learning and scientific computing (SciMARL) for modeling and control of complex flow-structure interactions. I will juxtapose successes and failures and argue that the proper fusion of fluid mechanics knowledge and AI expertise is essential to advance scientific frontiers.

12.30-13.00 - *"Optimizing Airborne Wind Energy with Reinforcement Learning"* - **Antonio Celani**

Airborne Wind Energy is a lightweight technology that allows power extraction from the wind using airborne devices such as kites and gliders, where the airfoil orientation can be dynamically controlled in order to maximize performance. The dynamical complexity of turbulent aerodynamics makes this optimization problem unapproachable by conventional methods such as classical control theory, which rely on accurate and tractable analytical models of the dynamical system at hand. Here we propose to attack this problem through Reinforcement Learning, a technique that -- by repeated trial-and-error interactions with the environment -- learns to associate observations with profitable actions without requiring prior knowledge of the system. We show that in a simulated environment Reinforcement Learning finds an efficient way to control a kite so that it can tow a vehicle for long distances. The algorithm we use is based on a small set of intuitive observations and its physically transparent interpretation allows to describe the approximately optimal strategy as a simple list of maneuvering instructions.

13.00-14.30 - LUNCH

14.30-15.00 - *"Learned navigation of smart active particles"* **- Holger Stark**

Biological microswimmers move or need to navigate in complex environments such as porous soil or landscapes of external cues. For all the artificially generated microswimmers it is a challenge to mimic navigation strategies from biology. Nevertheless, it is of utmost interest to fully explore how learned navigation takes place.

The talk addresses recent work where we look at optimal steering of active particles along the fastest path in a potential landscape and show how a smart active particle learns optimal steering via a reinforcement-learning strategy [1]. We also show how reinforcement learning helps to cope with noise.

While so far the swimmer senses its local position, we now explore the case, where the microswimmer senses direction and distance, which might have more relevance for biology. Finally, we also present first results for learned optimal navigation under different flow conditions.

[1] E. Schneider and H. Stark, EPL 127, 64003 (2019).

15.00-15.30 - *"Physical and data-driven modeling for Earth observation"* **- Bertrand Le Saux**

The European Space Agency (ESA) Φ-lab investigates the use of new Artificial Intelligence methods which can accelerate and transform Earth observation and Earth system modeling. We present a few use-cases in Earth sciences where the physical modeling of phenomena (e.g., by means of fluid dynamics of the atmosphere) could be combined and improved by machine learning based on observations from satellites and meteorological records. We will discuss cloud dynamics, rainfall forecasting, evolution of cyclonic systems, etc.

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15.30-16.00 - *"Modeling and controlling turbulent flows through deep learning"* - **Ricardo Vinuesa**

The advent of new powerful deep neural networks (DNNs) has fostered their application in a wide range of research areas, including more recently in fluid mechanics. In this presentation, we will cover some of the fundamentals of deep learning applied to computational fluid dynamics (CFD). Furthermore, we explore the capabilities of DNNs to perform various predictions in turbulent flows: we will use convolutional neural networks (CNNs) for non-intrusive sensing, i.e. to predict the flow in a turbulent open channel based on quantities measured at the wall. We show that it is possible to obtain very good flow predictions, outperforming traditional linear models, and we showcase the potential of transfer learning between friction Reynolds numbers of 180 and 550. We also discuss other modeling methods based on autoencoders (AEs) and generative adversarial networks (GANs), and we present results of deep-reinforcement-learning-based flow control.

16.00-16.30 - COFFEE BREAK

16.30-16.40 - *"Reinforcement learning of optimal active particle navigation"* - **Mahdi Nasiri**

In sufficiently complex environments, there is no simple way to determine the fastest route of an active particle that can freely steer towards a given target. In fact, while classical path planning algorithms (e.g. A*, Dijkstra) tend to fail to reach the global optimum, analytical approaches are incapable of handling generic complex environments. In this talk we will present a policy gradient-based deep reinforcement learning method that employs a hybrid continuum-based representation of the environment and allows, for the first time, to determine the asymptotically optimal path in complex environments. Our results provide a key step forward towards a universal path planner for future intelligent active particles and nanorobots with potential applications in microsurgery as well as in drug and gene delivery.

16.40-16.50 - *"Optimal navigation strategies in complex and noisy environments"* **- Lorenzo Piro**

Finding the fastest path to a desired destination is a vitally important task for microorganisms moving in a fluid flow. We address this problem by designing new navigation strategies that allow for travel time optimization of microscopic self-propelled particles in complex and noisy environments. Inspired by the control maps provided by the stochastic optimal control framework, here we design new simple strategies that allow microscopic self-propelled particles to adapt their motility in response to external stimuli such as light gradients, mimicking the tactic behaviors observed in a number of natural and artificial microswimmers. This is in contrast to strategies relying on the results of optimal control theory or machine learning algorithms and which require control over the microswimmer motion via external feedback loops. Remarkably, even though the strategies we propose rely on simple principles, they show arrival time statistics strikingly similar to those obtained from stochastic optimal control theory, as well as performances that are robust to environmental changes and strong fluctuations. These features, as well as their applicability to more general optimization problems such as navigation on curved manifolds, make these strategies promising candidates for the realization of optimized semi-autonomous navigation.

16.50-17.00 *"Data reconstruction of turbulent flows with Gappy POD and Generative Adversarial Networks"* - **Tianyi Li**

How to improve data assimilation of turbulent flows is an open question in different fields, from geophysics and astrophysics to several engineering applications. Difficulties of filling the missing data mainly depend on two factors: the complexity of the data and the large spatio-temporal sparsity of typical measurements. In this work we present a comparative study between Gappy POD and Deep Generative Adversarial Network (GAN) for the reconstruction of a turbulent flow in the presence of rotation. Results show that for random gappiness with moderate area, both methods give satisfying reconstruction. However, for large random gappiness and a square gap where much coherent information is missing, not only GAN reconstruction has smaller L2 error than Gappy POD, but also the turbulent statistical properties of higher-order observables are reproduced much better by the GAN reconstruction. As we show, this can be explained by the presence of adversarial loss during the GAN training. This work was supported by the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (Grant Agreement No. 882340).

17.00-17.30 *"Generalizable Data-augmented Turbulence Modeling using Learning and Inference assisted by Feature-space Engineering (LIFE)"* - **Karthik Duraisamy**

This talk will cover a set of approaches that are targeted towards the goal of developing generalizable data-augmented turbulence models. The critical components of this approach are: (1) Imposition of strictly necessary physical constraints; (2) Maintaining consistency between the learning and prediction environments; (3) Tightly-coupled inference and learning by constraining the augmentation to be learnable throughout the inference process; (4) Meticulous design of a parsimonious set of physics-informed, locally non-dimensional, and bounded features while promoting construction of a one-to-one features-to-augmentation map;(5) Localized learning to maintain explicit control over feature space to sensitize the augmentation function behavior only in the vicinity of available data. This approach is applied in the context of transition and turbulence modeling, and demonstrates the potential to yield generalizable models with sparse data. Perspectives will also be provided towards a complete framework of turbulence modeling.

17.30-18.00 *"Using machine learning in geophysical data assimilation (some of the issues and some ideas)"* **- Alberto Carrassi**

In recent years, data assimilation, and more generally the climate science modeling enterprise have been influenced by the rapid advent of artificial intelligence, in particular machine learning (ML), opening the path to various forms of ML-based methodology.

In this talk we will schematically show how ML can be included in the prediction and DA workflow in three different ways. First, in a so-called "non-intrusive" ML, we will show the use of supervised learning to estimate the local Lyapunov exponents (LLEs) based exclusively on the system's state [1]. In this approach, ML is used as a supplementary tool, added to the given physical model. Our results prove ML is successful in retrieving the correct LLEs, although the skill is itself dependent on the degree of local homogeneity of the LLEs on the system's attractor.

In the second and third approach, ML is used to substitute fully [4] or partly [5]a physical model with a surrogate one reconstructed from data. Nevertheless, for high-dimensional chaotic dynamics such as geophysical flows this reconstruction is hampered by (i) the partial and noisy observations that can realistically be gathered, (ii) the need to learn from long time series of data, and (iii) the unstable nature of the dynamics. To achieve such inference successfully we have suggested to combine DA and ML in several ways. We will show how to unify these approaches from a Bayesian perspective, together with a description of the numerous similarities between them [2,3] . We will show that the use of DA in the combined approach is pivotal to extract much information from the sparse, noisy, data. The full surrogate model achieves prediction skill up to 4 to 5 Lyapunov time, and its power spectra density is almost identical to that of the original data, except for the high-frequency modes which are not well captured [4]. The ML-based parametrization of the unresolved scales in the third approach studied using a coupled atmosphere-ocean model and again the use of coupled DA [5] is also extremely skilful. The combined DA-ML method makes it possible to exploit the data information from one model compartment (e.g., the ocean) to the other (e.g., the

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atmosphere).

18.00-18.30 *"Optimal Microswimmer Navigation"* - **Benno Liebchen**

Finding the fastest route to a target is a very well explored problem for macroscopic agents like ships, robots or airplanes which often move with a preferred speed but can freely steer.
In contrast, the quest on how to steer a microswimmer to optimally reach a predefined target involves new challenges due to the presence of significant fluctuations, hydrodynamic interactions and "strong" environments.
In this talk, I'll discuss both theoretical and machine-learning based advances en route towards a universal path planner for microswimmers. The talk first discusses a variational principle which determines the optimal path for self-propelled particles and creates a surprising link to classical ray optics by establishing Fermat's principle and Snell's law for microswimmers (which can follow a similar path as light in metamaterials).
We proceed by discussing the influence of hydrodynamic interactions and fluctuations on optimal microswimmer navigation, which can qualitatively change the required navigation strategy. Finally, we use our theoretical results to benchmark a generic machine learning based approach, which we have developed to find the optimal navigation strategy even in environments which are too complex to allow for analytical (or classical algorithmic) solutions.

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9.30-10.00 *"Data-driven manifold dynamics"* - **Michael Graham**

The success of many machine learning applications is often attributed to the "manifold hypothesis", the idea that many nominally very high-dimensional data sets actually reside on or near a manifold of much lower dimension within the ambient space. In applications such as fluid mechanics that are governed by dissipative PDE we expect this hypothesis to be strictly valid, as dissipation smooths out small scales leading the long-time dynamics to lie on a finite-dimensional invariant manifold sometimes called the inertial manifold. We describe a data-driven reduced order modeling method that (1) estimates manifold dimension and determines a coordinate representation of the manifold using an autoencoder, and (2) learns an ODE describing the dynamics in these coordinates, using the so-called neural ODE framework. With the ODE representation, data can be widely spaced and no time derivatives of data are required. We apply this framework to spatiotemporal chaos in the Kuramoto-Sivashinsky equation (KSE), chaotic bursting dynamics of Kolmogorov flow, and transitional turbulence in plane Couette flow, finding dramatic dimension reduction while still yielding good predictions of short-time trajectories and long-time statistics. An important extension of this approach emerges from the recognition that for a general manifold, no single intrinsic global Cartesian coordinate representation can be found. In the language of topology an "atlas" of overlapping local coordinate representations, or "charts", must be used. We use this framework to represent nonlinear dynamics of dissipative PDEs on manifolds of intrinsic dimension.

10.00-10.30 - *"Optimal policies for olfactory search in turbulent flows"* - **Robin Heinonen**

In many practical scenarios, a flying insect must search for the source of an emitted cue which is advected by the atmosphere. On the macroscopic scales of interest, turbulence tends to mix the cue into patches of relatively high concentration over a background of very low concentration, so that the insect will only detect the cue intermittently and cannot rely on chemotactic strategies which simply climb the concentration gradient. In this work, we cast this search problem in the language of a partially observable Markov decision process (POMDP) and use the Perseus algorithm to compute strategies that are near-optimal with respect to the arrival time. We test the computed strategies on a large two-dimensional grid, present the resulting trajectories and arrival time statistics, and compare these to the corresponding results for several heuristic strategies, including (space-aware) infotaxis, Thompson sampling, and QMDP. We find that the near-optimal policy found by our implementation of Perseus outperforms all heuristics we test by several measures. We discuss additionally the choice of initial belief, the robustness of the policies to changes in the environment, and the benefits (and pitfalls) of employing a reward shaping function.

10.30-11.15 COFFEE BREAK

11.15-11.45 *"Searching for a source in turbulence: from heuristics to deep reinforcement learning"* **- Aurore Loisy**

Tracking down a source of scalar in a turbulent flow is hard. To assess the performance of possible strategies, Vergassola et al. (Nature, 2007) designed a POMDP (partially observable Markov decision process) that mimics these challenging searching conditions in a computation-friendly environment. In this POMDP, the agent must find a stationary target (the source) hidden in a grid world using stochastic partial observations (odor detection events). Good strategies must ensure that the source is always found, but to be optimal they must also minimize the duration of the search. In this talk, I will discuss a good heuristic strategy, the popular "infotaxis" (Vergassola et al., Nature 2007), and I will show how deep reinforcement learning can find (near) optimal strategies that are able to beat it.

11.45-12.15 - Bethany Lusch **TBA**

12.14-12.45 "*Vector-cloud neural network for nonlocal constitutive modeling*" **- Heng Xiao**

Partial differential equations (PDEs) have been used to represent field-to-field mapping in science and engineering. However, in many cases the PDEs are expensive or impossible to solve, e.g., due to stiff terms or unclosed terms. Recently, neural networks have been explored to represent such field-to-field mapping, which are referred to as "neural operators". In this talk, we present a neural operator called vector-cloud neural network (VCNN), which maps between fields represented by an arbitrary set of points. We demonstrate its potential applications in turbulence modeling. A comparison to graphical neural networks (GNN) is also discussed. We highlight the frame-invariance of the neural operators and its importance for physical modeling.

12.45-14.15 LUNCH

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14.15-14.45 *"Neural Corrections for Fast Fluid Flow Solvers"* **- Gianluca Iaccarino**

Applications of machine learning techniques to physics applications are gaining popularity by providing solution process acceleration, super-resolution, equation discovery, etc. Different flavors of data driven techniques have been proposed in the literature; we focus on hybrid approaches in which an existing grid-based numerical technique for the governing equations is augmented with a neural network correction. It is unclear if these approaches provide improvements over the baseline numerical solver by approximating local subgrid-scale dynamics, by incorporating long-range spatial/temporal correlations or by introducing high-order-like solution reconstructions. Furthermore, it is often difficult to assess how different aspects of the training pipeline affect the quality of the neural correction and its generalizability. In this work we investigate the issues above using both the Burgers and the Navier-Stokes equations.

14.45-15.15 *"Learning from Interactions between Models and Differentiable Physics"* **- Kiwon Um**

Finding solutions to partial differential equations (PDEs) is a crucial task in all scientific and engineering disciplines. Recently, machine learning techniques have been demonstrating their great capacity for a variety of PDE problems in improving conventional numerical solvers. In this talk, the speaker will discuss a novel machine learning approach that adopts a differentiable physics framework to address the limitation of conventional PDE solvers. This framework allows trainable models to interact with PDE solvers in its learning process such that the models can learn better particularly for recurrent learning tasks. Aiming for reducing numerical errors of given iterative PDE solvers, different learning approaches will be discussed and compared.

15.15-15.45 *"Choosing parameters for successful reservoir computing"* **- Kristian Gustafsson**

An echo state network is a type of reservoir computer that often performs well on time series prediction tasks. However, it is in most cases not clear how to best choose the parameters of the network for successful prediction. Using methods of dynamical systems, we identify two key parameter groups for prediction performance. We find that the parameter region where prediction is successful, is heavily influenced by the time series to be predicted. We explain how these regions of successful reservoir computing emerge for a couple of cases.

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15.45-16.30 COFFEE BREAK

16.30-16.40 *"Optimal Control tools to minimize dispersion in chaotic flows"* **- Chiara Calascibetta**

We develop optimal and quasi-optimal strategies to control Lagrangian objects navigating in 2d stochastic and complex flows. We consider the problem of minimizing the dispersion rate of a couple of autonomous explorers moving into the complex fluid environment. Starting from the optimal solutions derived in control theory, we find approximated solutions that could be applied also under less restrictive conditions as, e.g., in the presence of partial observability. We are going to compare hard-wired policies resulting from different approximated solutions of the optimal control theory against strategies obtained by data-driven tools based on Reinforcement Learning.
This work was supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant Agreement No. 882340).

[1] Optimal Control tools to minimize dispersion in chaotic flows, Calascibetta Chiara, Biferale Luca, Borra Francesco, Celani Antonio, Cencini Massimo, in preparation 2022.

16.40-16.50 *"Active gyrotactic stability of microswimmers using hydro-mechanical signals"* **- Navid Mousavi**

Many plankton species undergo daily vertical migration to large depths in the turbulent ocean. To do this efficiently, the plankton can use a gyrotactic mechanism, aligning them with gravity to swim downwards or against gravity to swim upwards. Many species show passive mechanisms for gyrotactic stability. For example, bottom-heavy plankton tend to align upwards. This is efficient for upward migration in quiescent flows, but it is often sensitive to turbulence which upsets the alignment. Here we suggest a simple, robust active mechanism for gyrotactic stability, which is only lightly affected by turbulence and allows alignment both along and against gravity. We use a model for a plankton that swims with a constant speed and can actively steer in response to hydrodynamic signals encountered in simulations of a turbulent flow. Using reinforcement learning, we identify the optimal steering strategy. By using its setae to sense its settling velocity transversal to its swimming direction, the swimmer can deduce information about the direction of gravity, allowing it to actively align upwards. The mechanism leads to a rate of upward migration in a turbulent flow that is of the same order as in quiescent flows, unless the turbulence is very vigorous. In contrast, passive swimmers with typical parameters of copepods show much smaller upward velocity in turbulence. Settling may even cause them to migrate downwards in vigorous turbulence.

Reference

Qiu, J., Mousavi, N., Zhao, L., & Gustavsson, K. (2022). Active gyrotactic stability of microswimmers using hydro-mechanical signals. Physical Review Fluids, 7(1), 014311.

16.50-17.00 *"A data-driven approach for second-order thermal turbulence modeling"* - **Matilde Fiore**

Non-isothermal turbulent flows govern many phenomena of industrial and academic interest. Despite the continuous increase of computational resources for the direct and the large-eddy simulation of turbulence, the Reynolds Averaged Navier-Stokes (RANS) approach is still considered the workhorse of industrial research, and the accurate modeling of the turbulent statistics remains essential to retrieve the correct thermal and momentum fields in a wide range of problems.

Data-driven techniques open new perspectives in turbulence modeling as they ease the exploitation and interpretation of big datasets and the calibration of complex models. This work presents a data-driven approach to improve a Differential Transport Heat Flux Model (DTHFM), with special attention to its accuracy for low Prandtl number fluid flows. Improving the DTHFM requires the integration of sub-models for the individual budget terms and the resolution of the transport equations at each model evaluation.

The proposed approach consists of three main steps. First, an inverse problem is solved to compute the correction term at each point of the database of interest. Then, a correlation analysis is carried out to interpret the physical meaning of the correction and to assign it to the fundamental mechanisms regulating the evolution of thermal turbulence. Finally, the results of this analysis guided the mathematical formulation of the modeled correction and the design of an Artificial Neural Network (ANN) model to predict its unclosed coefficients. The results obtained with non-isothermal turbulent channel flows show that the corrective model is well parametrized and the heat flux predictions significantly improve, especially at low Prandtl numbers.

17.00-17.10 *"Reinforcement learning for pursuit and evasion of microswimmers at low Reynolds number"* - **Francesco Borra**

Many aquatic organisms can exploit hydrodynamic information to navigate, hunt their preys and escape from predators. Abstracting away from specific biological mechanisms, we study an adversarial model of two microswimmers engaging in a pursue-evasion (zero-sum) game while immersed in an idealized low-Reynolds-number aquatic environment. The agents have only access to information obtained from hydrodynamic disturbances generated by their opponent, which provide some cues about its swimming direction and position. They can only perform simple maneuvers: turn left, right or go straight. The goal of the predator/pursuer is to capture the evader/prey in the shortest possible time. Conversely, the prey tries to avoid it or at least delay it as much as possible. We let the agents discover their strategies by means of an actor-critic Reinforcement Learning algorithm. We show that the agents are able to find efficient and a-posteriori physically explainable strategies which non-trivially exploit both the dynamics and the hydrodynamic signals. Our study provides a proof-of-concept for the use of Reinforcement Learning to rationalize prey-predator interactions in aquatic environments, and is potentially relevant to artificial agents applications.

17.10 -17.40 *"Reliability and generalization of machine-learning predictions: two examples"* - **Onofrio Semeraro**

The breakthrough of machine-learning based applications is revolutionizing scientific computing; however, despite numerous successful examples -- mainly based on deep neural network -- the relative simplicity of applications of these tools is flawed by numerous issues that are too often overlooked such as generalizability of the models, lack of guarantees or case dependency. Increasing the size of the dataset of training, as well as relying on deeper and more expressive architectures do not necessarily guarantee a solution for these issues, while leading to longer training and thus to higher computational costs. The potential lack of robustness of these predictions is often mitigated by prior knowledge of physical constraints, when available. Here, we propose two different examples where different paths are undertaken.

In the first example, we will consider Long-Short Term Memory neural networks and thoroughly investigate the impact of the training set, its structure and some issues relating the use of memory gates on the quality of the long-term prediction. Inspired by ergodic theory, we analyze the amount of data sufficient for a priori guaranteeing a faithful model of the physical system, relying on a proper dataset design. We show how an informed design of the training set, based on invariants of the system and the structure of the underlying attractor, significantly improves the resulting models, opening up avenues for research within the context of active learning, towards the paradigm-shift currently dubbed as “data-centric machine learning”.

In the second example, we will discuss graph neural networks (GNN) and deploy them for the closure of turbulence models within the context of Reynolds-Averaged Navier-Stokes (RANS)

equations. GNNs have a strong potential due to their peculiarities: this architecture is characterized by complex multi-connected nets of nodes that can be provided as input and easily adapted to unstructured mesh for computational fluid mechanics and data-driven modeling. A supervised learning closure term for RANS equation is trained on data stacked at different Reynolds numbers from simulations of wakes developing past a cylinder, and later applied on different geometries.
The results provide evidence on the extent to which it is possible to parametrize the GNN models and perform operator learning, leveraging the mesh independency.
These works are performed in collaboration with Michele Alessandro Bucci, Thibault Monsel, Michele Quattromini, Sergio Chibbaro and Lionel Mathelin.

17.40 -18.10 *"Machine Learning and Feedback Microscopy"* **- Frank Cichos**

Local dynamic temperature fields generated by an optical pumping of plasmonic nanostructures allow to manipulate liquids, particles and molecules in microfluidic geometries. Combined with real-time image analysis such manipulative actions provide a powerful tool for a feedback control of microscopic samples.
We combine these feedback control approaches to explore experimentally the application of machine learning techniques in the feedback control process. We demonstrate delay induced non-linear dynamical systems of active particles that provide memory. Such active particles resemble a physical realization of recurrent nodes. Coupling these nodes creates reservoirs that can be used for time series prediction and active particle control itself. We further report on reinforcement learning studies applied to the control of active particles investigating the influence of Brownian motion on the learning process. Extensions to microfluidic control are discussed.

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9.30-10.00 *"FourCastNet: A Data-driven Model for High-resolution Weather Forecasts using Adaptive Fourier Neural Operators"* **- Peter Harrington**

FourCastNet, short for Fourier Forecasting Neural Network, is a global data-driven weather forecasting model that provides accurate short to medium-range global predictions at 25km resolution. FourCastNet accurately forecasts high-resolution, fast-timescale variables such as the surface wind speed, precipitation, and atmospheric water vapor. It has important implications for planning wind energy resources, predicting extreme weather events such as tropical cyclones, extra-tropical cyclones, and atmospheric rivers. FourCastNet matches the forecasting accuracy of the ECMWF Integrated Forecasting System (IFS), a state-of-the-art Numerical Weather Prediction (NWP) model, at short lead times for large-scale variables, while outperforming IFS for variables with complex fine-scale structure, including precipitation. FourCastNet generates a week-long forecast in less than 2 seconds, orders of magnitude faster than IFS. The speed of FourCastNet enables the creation of rapid and inexpensive large-ensemble forecasts with thousands of ensemble-members for improving probabilistic forecasting. We discuss how data-driven deep learning models such as FourCastNet are a valuable addition to the meteorology toolkit to aid and augment NWP models.

10.00-10.30 *"Symbolic regression as example for explainability "* **- Markus Abel**

Explainability of artificial intelligence is increasingly important: consequences of the application of an algorithm on critical topics must be quantitatively assessed and explained in a human understandable way. For systems governed by equations, like fluids or nonlinear systems in general, one way consists of the determination of underlying equations for subsequent further analysis. We show the use of symbolic regression with subsequent bifurcation analysis with AUTO, on a general example of system change, and eventually explain failure of methods, in relation to the data requirements.

10.30-11.15 COFFEE BREAK

11.15-11.45 *"Steering undulatory microswimmers in a moving fluid through reinforcement learning"* **- Jérémie Bec**

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A new model of microswimmer is introduced to investigate locomotion strategies based on the sinusoidal undulation of a slender body. These active particles are then embedded in a prescribed fluid flow in which their swimming undulations have to compete with the drifts, strains and deformations inflicted by the outer velocity field. Such an intricate situation, where swimming and navigation are tightly bonded, is addressed using reinforcement learning. It is shown that the displacement strategy of the microswimmers can be optimized using Q-learning. Still, such an approach rapidly becomes rather expensive because of the highly chaotic character of the swimmers dynamics yielding a strong variability in the algorithm convergence. Results however lead to construct an ensemble of admissible strategies whose robustness is addressed varying several physical parameters of the problem and applied to swimmers in non-stationary flows.

11.45-12.15 *"Lagrangian Large Eddy Simulations via Physics Informed Machine Learning"*
Michael Chertkov

High Reynolds Homogeneous Isotropic Turbulence (HIT) is fully described within the Navier-Stokes (NS) equations, which are notoriously difficult to solve numerically. Engineers, interested primarily in describing turbulence at reduced but sufficiently large range of resolved scales, have designed heuristics, known under the name of Large Eddy Simulation (LES). LES is described in terms of the evolving in time Eulerian velocity field defined over the points of a constant (that is not evolving in time) spatial grid with the mean-spacing correspondent to the resolved scale. These classic Eulerian LES depend on assumptions about effects of sub-grid scales on the resolved scales. We take an alternative approach and design novel LES heuristics stated in terms of Lagrangian particles moving with the turbulent flow. Our Lagrangian LES, thus L-LES, is described by equations, generalizing equations of the weakly compressible Smooth Particle Hydrodynamics (SPH), with extended parametric and functional freedom which is then resolved/fixed via Machine Learning (ML) training on Lagrangian data from a Direct Numerical Simulation (DNS) of the NS equations. The L-LES framework includes parameters which are explainable in clear physical terms, e.g. parameters describing effects of eddy-diffusivity and smoothing kernels, and Neural Networks (NN) to represent effects of smaller (unresolved) scales and relations between velocity and pressure fields evaluated at the particle positions in a functional form. We utilize modern methodology of Differentiable Programming (DP) and Deep NN to train the parametric and functional degrees of freedom. We experiment with loss functions of different types, including physics-informed ones accounting for statistics of Lagrangian particles. We show, through a series of diagnostic tests, that the developed L-LES allows to describe turbulence from a unique perspective that is inaccessible from Eulerian LES. We also show that the L-LES is capable to reproduce Lagrangian and Eulerian statistics of the flow at the resolved scales. This is a joint work of LANL and UArizona teams (with Y. Tian, M. Woodward, M. Stepanov, C. Hyett, C. Fryer and D. Livescu).

12.15-12.45 "*Towards a Numerical Proof of Turbulence Closure*" - **Federico Toschi**

The development of turbulence closure models, parametrizing the influence of small non-resolved scales on the dynamics of large resolved ones, is an outstanding theoretical challenge with vast applicative relevance. We present a closure, based on deep recurrent neural networks, that quantitatively reproduces, within statistical errors, Eulerian and Lagrangian structure functions and the intermittent statistics of the energy cascade, including those of subgrid fluxes. To achieve high-order statistical accuracy, and thus a stringent statistical test, we employ shell models of turbulence. Our results encourage the development of similar approaches for 3D Navier-Stokes turbulence.

12.45-14.15 - LUNCH

14.15-14.45 "*Learning to navigate complex environments*" - **Massimo Vergassola**

Living systems face the challenge of navigating natural environments shaped by non-trivial physical mechanisms. Notable examples are provided by long-distance orientation using airborne olfactory cues transported by turbulent flow, the tracking of surface-bound trails of odor cues, and flight in the lowest layers of the atmosphere. Terrestrial animals, insects, and birds have evolved navigation strategies that accomplish the above tasks with an efficiency that is often surprising and yet unmatched by human technology. Indeed, robotic applications for olfactory sniffers and unmanned aerial vehicles face similar challenges for the automated location of explosives, chemical, and toxic leaks, as well as the monitoring of biodiversity, surveillance, disaster relief, cargo transport, and agriculture. The interdisciplinary interplay between biology, physics, and robotics is key to jointly advancing fundamental understanding and technology. I shall review the above natural phenomena, then discuss the physics that constrains and shapes the navigation tasks, how machine-learning methods are brought to bear on those tasks, and conclude with the relevant strategies of behavior and open issues.

14.45-15.15 "*Reconstruction and preparation of turbulent states*" - **Patricio Clark di Leoni**

Workshop

Challenges and Benchmarks for quantitative AI in Complex Fluids and Complex Flows

Centro Ricerche Enrico Fermi

Piazza Viminale 1, Rome, Italy 6-8 JULY 2022

Reconstructing realizations of turbulent flows out of incomplete and noisy data is challenging in many applications. In this talk we show two ways for reconstructing high Reynolds number flows, one based on a data assimilation technique called nudging, which seeks to synchronize the flow's evolution to some given data, and the other based on Physics-Informed Neural Networks, which combine the power of neural networks with physical knowledge of the problem. We show results from both synthetic and experimental flows. Finally, we show how to prepare turbulent states where the only information provided is on the statistics of the flow.

15.15-15.25 *"DA for a new generation of sea-ice model"*- .**Yumeng Chen**

Data assimilation (DA) combines observations with model forecasts to improve the trajectory and/or the parameters of numerical models. Recently, DA shows flourishing applications for the Artic sea-ice, thanks primarily to the increasing satellite observations. Together with better observations, sea-ice models have undergone a substantial change of paradigm.

Instead of treating the sea ice as viscous fluid, the recently developed, neXtSIM, uses a novel Maxwell-Elasto-Brittle (MEB) rheology treating the sea ice as elastic and viscous materials. For better efficiencies, the neXtSIM adopts a Lagrangian grid where the position and number of grid points change with time. This sets challenges for ensemble DA methods where each ensemble member will have a different mesh.

We will show the application of the EnKF when the analysis is performed on a given fixed-in-time reference mesh. Our experiments demonstrate that DA can improve seasonal sea ice forecasting skills in the novel sea ice model during the Arctic winter by assimilating the sea ice concentration and thickness from satellite data.

Nevertheless, the Lagrangian model presents issues with coupling to atmosphere and ocean models. To overcome this issue for climate simulations, neXtSIM_DG adopting discontinuous Galerkin method on Eulerian grids is under development. The newly developed neXtSIM_DG provides opportunities to improve sea ice prediction by inferring the model parameters and exploiting the numerical features of DG methods with state-of-the-art DA methods. In our talk, we will show an overview of these ideas.

15.25-15.35 *"Machine learning for optimal control in an axial compressor"*- **Mohamed Elhawary**

Active flow control via air-jets is one the prominent techniques for mitigating rotating stall in axial compressors. In this study, the control parameters of a set of air-jets is optimized using Deep Neural Networks (DNNs) and Genetic Algorithms (GAs). The control configuration consists of 20 pairs of air-jets that are positioned circumferentially upstream the leading edge of the rotor of an axial compressor (CME2). Three control parameters are investigated, namely the injection velocity, the injection angle, and the number of injector pairs. The performance of the compressor under control is evaluated in terms of the surge margin increase and the power balance at 3200 RPM, 4500 RPM, and 6000RPM (Reynolds number..). A set of experiments is utilized for training the deep neural network model, then a genetic algorithm is employed for optimization. The results show great capabilities of the DNN model in predicting the performance of the compressor with an R_squared error higher than 90% for training and testing data. Based on the optimization process, additional experiments have been carried-out at 3200 RPM to explore the optimal injection angle as well as testing the extrapolation capabilities of the DNN model.

15.35-16.20 COFFEE BREAK

16.20-16.50 *"Comparative analysis of machine learning methods for active flow control"*- **Miguel Alfonso Mendez**

Machine learning frameworks such as Genetic Programming (GP) and Reinforcement Learning (RL) are gaining popularity in flow control. This talk presents a comparative analysis of the two, bench-marking some of their most representative algorithms against global optimization techniques such as Bayesian Optimization (BO) and Lipschitz global optimization (LIPO). Three test cases of growing complexity are analyzed. These are (1) the stabilization of a nonlinear dynamical system featuring frequency cross-talk, (2) the wave cancellation from a Burgers' flow and (3) the drag reduction in a cylinder wake flow. A connection to classic control theory is discussed, along with their differences in exploration versus exploitation and their balance between `model capacity' in the control law definition versus `required complexity'. We believe that such a comparison opens the path towards hybridization of the various methods, and we offer some perspective on their future development in the literature of flow control problems.

16.50-17.20 *"Interpreted machine learning in fluid dynamics: explaining relaminarization events in wall-bounded shear flows"* **Moritz Linkmann**

Machine Learning (ML) is becoming increasingly popular in fluid dynamics. Powerful ML algorithms such as neural networks or ensemble methods are notoriously difficult to interpret. Here, we introduce the novel Shapley additive explanations (SHAP) algorithm (Lundberg & Lee, Advances in Neural Information Processing Systems, 2017, pp. 4765–4774), a game-theoretic approach that explains the output of a given ML model in the fluid dynamics context. We give a proof of concept concerning SHAP as an explainable artificial intelligence method providing useful and human-interpretable insight for fluid dynamics. To show that the feature importance ranking provided by SHAP can be interpreted physically, we first consider data from an established low-dimensional model based on the self-sustaining process (SSP) in wall-bounded shear flows, where each data feature has a clear physical and dynamical interpretation in terms of known representative features of the near-wall dynamics, i.e. streamwise vortices, streaks and linear streak instabilities. SHAP determines consistently that only the laminar profile, the streamwise vortex and a specific streak instability play a major role in the prediction. We demonstrate that the method can be applied to larger fluid dynamics datasets by a SHAP evaluation on plane Couette flow in a minimal flow unit focussing on the relevance of streaks and their instabilities for the prediction of relaminarization events. Here, we find that the prediction is based on proxies for streak modulations corresponding to linear streak instabilities within the SSP. That is, the SHAP analysis suggests that the break-up of the self-sustaining cycle is connected with a suppression of streak instabilities.

17.20-17.50 "*Machine Learning for Climate and Weather Prediction*" **Edward Ott**

This talk will discuss an approach to the application of machine learning to Earth climate and weather prediction. This approach [1] uses a hybrid parallel architecture combining a reservoir computing component with a conventional knowledge-based component. Key issues discussed include scalability to large spatiotemporally complex heterogeneous situations, stability [2], and (in the case of climate) nonstationary dynamics [3]. Current numerical test results [4], along with future plans and prospects, will be presented.

[1] A. Wikner et al., Chaos, 053111 (2020); J. Pathak et al., PhysRevLett, 024102 (2018); J. Pathak et al., Chaos, 041101 (2018).
[2] Z. Lu, B. Hunt, E. Ott, Chaos, 061108 (2018).
[3] D. Patel et al., Chaos, 033149(2021).
[4] T. Arcomano et al., J. Advances in Modeling Earth Systems, e2021MS002712 (2022); T. Arcomano et al., J. Geophys. Res. Lett., e2020GL87776 (2020).

17.50-18.00 CLOSING