Symposium AI in (Bio-)Physics (SYAI)

jointly organised by
the Biological Physics Division (BP),
the Chemical and Polymer Physics Division (CPP),
the Dynamics and Statistical Physics Division (DY), and
the Physics of Socio-economic Systems Division (SOE)

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Artificial intelligence is revolutionizing scientific research, including the study of biophysical systems. The symposium will explore how AI and machine learning can enhance biophysics research, with applications ranging from predictive modeling of biomolecular interactions and high-throughput data analysis to the development of machine-learned force fields and artificial scientific discovery. The goal of this symposium is to create a dynamic forum for scientific exchange in this rapidly developing field, providing novices with a valuable head start while helping experts stay at the forefront of cutting-edge developments. The conceptual nature of AI-powered research approaches will make the discussed topics highly relevant to a broad audience.

Overview of Invited Talks and Sessions

(Lecture hall H1)

Invited Talks

SYAI 1.1	Thu	9:30–10:00	H1	**Predicting interaction partners and generating new protein sequences using protein language models** — •Anne-Florence Bitbol
SYAI 1.2	Thu	10:00–10:30	H1	**Realizing Schrödinger's dream with AI-enabled molecular dynamics** — •Alexandre Tkatchenko
SYAI 1.3	Thu	10:30–11:00	H1	**Emergent behavior of artificial intelligence** — •Steffen Rulands
SYAI 1.4	Thu	11:15–11:45	H1	**AI in medical research - navigating complexity with AI** — •Daniel Truhn
SYAI 1.5	Thu	11:45–12:15	H1	**Computational Modelling of Morphogenesis** — •Dagmar Iber

Sessions

SYAI 1.1–1.5	Thu	9:30–12:15	H1	**AI in (Bio-)Physics**

SYAI 1: AI in (Bio-)Physics

Time: Thursday 9:30–12:15 Location: H1

Invited Talk SYAI 1.1 Thu 9:30 H1

Predicting interaction partners and generating new protein sequences using protein language models — •Anne-Florence Bitbol — École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

Protein sequences are shaped by functional optimization on the one hand and by evolutionary history, i.e. phylogeny, on the other hand. A multiple sequence alignment of homologous proteins contains sequences which evolved from the same ancestral sequence and have similar structure and function. In such an alignment, statistical patterns in amino-acid usage at different sites encode structural and functional constraints.

Protein language models trained on multiple sequence alignments capture coevolution between sites and structural contacts, but also phylogenetic relationships. I will discuss a method we recently proposed that leverages these models to predict which proteins interact among the paralogs of two protein families, and improves the prediction of the structure of some protein complexes. Next, I will show that these models can be used to generate new protein sequences from given protein families.

While multiple sequence alignments are very useful, their construction is imperfect. To address these limitations, we developed ProtMamba, a homology-aware but alignment-free protein language model based on the Mamba architecture, which efficiently uses long contexts. I will show that ProtMamba has promising generative properties, and is able to predict fitness.

Invited Talk SYAI 1.2 Thu 10:00 H1

Realizing Schrödinger's dream with AI-enabled molecular dynamics — •Alexandre Tkatchenko — Department of Physics and Materials Science, University of Luxembourg

The convergence between accurate quantum-mechanical (QM) models (and codes) with efficient machine learning (ML) methods seem to promise a paradigm shift in molecular simulations. Many challenging applications are now being tackled by increasingly powerful QM/ML methodologies. These include modeling covalent materials, molecules, molecular crystals, surfaces, and even whole proteins in explicit water (https://www.science.org/doi/abs/10.1126/sciadv.adn4397). In this talk, I attempt to provide a reality check on these recent advances.

In particular, I will introduce the recently developed SO3LR force field (https://doi.org/10.26434/chemrxiv-2024-bdfr0), trained on a diverse set of 4 million neutral and charged molecular complexes computed at the PBE0+MBD level of quantum mechanics, ensuring a comprehensive coverage of covalent and non-covalent interactions. SO3LR is characterized by computational and data efficiency, scalability to 200 thousand atoms on a single GPU, and reasonable to high accuracy across the chemical space of organic (bio)molecules. SO3LR is applied to study units of four major biomolecule types, polypeptide folding, and nanosecond dynamics of larger systems such as a protein, a glycoprotein, and a lipid bilayer, all in explicit solvent. Finally, I discuss the future challenges toward truly general molecular simulations by combining ML force fields with traditional atomistic models.

Invited Talk SYAI 1.3 Thu 10:30 H1

Emergent behavior of artificial intelligence — •Steffen Rulands — Arnold-Sommerfeld Center for Theoretical Physics, LMU München, Theresienstr. 37, 80333 München

Can artificially intelligent systems show emergent behavior that does not originate from the data they are trained on? This question is relevant for understanding the potential dangers and possibilities of powerful AI systems. In this talk, I will address this question from two different perspectives drawing on ideas from theoretical biophysics. First, I will show that neural networks exhibit an instability that gives rise to the emergent formation of structures independent of the training data. I will show how these structures aid the interpretation of data. In the second part of my talk, I will then draw on the biophysics of subcellular compartments and insect societies to demonstrate ways in which emergent behavior of artificially intelligent systems can facilitate and jeopardize deep learning.

15 min. break

Invited Talk SYAI 1.4 Thu 11:15 H1

AI in medical research - navigating complexity with AI — •Daniel Truhn — University Hospital Aachen, Germany

Modern artificial intelligence (AI) systems, including Large Language Models (LLMs) and advanced multimodal vision systems, are transforming clinical practice and medical research. This talk outlines how these technologies navigate complex medical challenges and enhance clinician efficiency. By showcasing practical applications, I demonstrate how AI empowers healthcare professionals to make better and faster decisions, ultimately improving patient outcomes.

Invited Talk SYAI 1.5 Thu 11:45 H1

Computational Modelling of Morphogenesis — •Dagmar Iber — Department of Biosystems Science and Engineering, ETH Zürich, Switzerland

Epithelia are fundamental building blocks of life, playing pivotal roles in morphogenesis and are at the origin of most cancers. This talk will explore epithelial organization across scales, from individual cell geometry to tissue-level architecture. I will introduce theoretical work that sheds light on long-standing, unexplained phenomena in epithelial cell organization, enabling the development of advanced 2D and 3D simulation tools. These tools allow for data-driven simulations of epithelial dynamics, advancing our understanding of both development and disease. Additionally, I will examine how chemical gradients drive precise epithelial patterning during development and demonstrate how their interplay with geometric and mechanical constraints shapes epithelial morphogenesis. Case studies include neural tube formation, lung branching morphogenesis, nephrogenesis, and bladder cancer progression. By integrating experimental insights with computational approaches, this work offers a comprehensive view of the mechanisms driving epithelial morphogenesis in health and disease.