

Final program of workshop "Advancing Scientific Machine Learning in Industry"

October 15-16, 2024
TU München – Institute for Advanced Study
Lichtenbergstrasse 2a, 85748 Garching

ABSTRACT

Scientific machine learning (SciML) has been taking the academic world by storm as an interesting blend of traditional scientific modelling with machine learning (ML) methodologies like deep learning. While traditional machine learning methodologies have difficulties with scientific issues like interpretability, and enforcing physical constraints, the blend of ML with numerical analysis and differential equations has evolved into a novel field of research which overcome these problems while adding the data-driven automatic learning features of modern machine learning. Many successes have already been demonstrated, with tools like physics-informed neural networks, universal differential equations, deep backward stochastic differential equation solvers for high dimensional partial differential equations, and neural surrogates showcasing how deep learning can greatly improve scientific modelling practice. Consequently, SciML holds promise for versatile application across a wide spectrum of scientific disciplines, ranging from the investigation of subatomic particles to the comprehension of macroscopic systems like economies and climates.

However, despite notable strides in enhancing the speed and accuracy of these methodologies, their utility in practical and specifically industrial settings remain constrained. Many domains within the scientific community still lack comprehensive validation and robustness testing of SciML approaches. This limitation is particularly pronounced when confronted with complex, real-world datasets emanating from interactions between machinery and environmental sensors as usually addressed in industry. Still if appropriately addressed, SciML with its promise to accelerate innovations and scientific discoveries by orders of magnitudes, offers unique opportunities to address the insatiable desire for faster and more accurate predictions in many fields.

This workshop is dedicated to exploring recent advancements in the implementation of SciML techniques. It convenes leading experts who are actively engaged in refining these methodologies to ensure their practical viability and scalability, particularly in industrial sectors where digital and physical components converge. Goal of the workshop is to produce a research roadmap for advancing scientific machine learning in industry, addressing application/industrialization challenges.

Organisers

This workshop is organized by TUM-IAS Hans Fischer senior fellow Wil Schilders and Siemens top innovator Dirk Hartmann.

Suggested accommodation

Close to the venue of the workshop are the Courtyard by Marriott hotel (https://www.marriott.com/en-us/hotels/muccg-courtyard-munich-garching/overview/) and the Stellaris Apartment hotel (https://www.stellaris-apartment.de/de/home).

How to reach TUM-IAS

https://www.ias.tum.de/ias/contact-directions/

Additional information

On the next page, the final program is provided. For additional and last minute information, please consult the web page of the Focus Group "Scientific Machine Learning":

https://www.ias.tum.de/ias/research-areas/advanced-computation-and-modeling/scientific-machine-learning/



Final program of workshop on

"Advancing Scientific Machine Learning in Industry"

Tuesday, October 15, 2024

10.00-10.30 Opening

Michael Molls (TUM-IAS), Hans Bungartz (TUM School of Computation, Information and Technology), Dirk Hartmann (Siemens) and Wil Schilders (TUM-IAS)

10.30-12.30 Industry presentations and challenges

- **■** Dirk Hartmann (Siemens), Scaling Machine Learning in Engineering Applications A far fetched dream or an achievable goal?
- Richard Szöke-Schuller (Simscale), Overcoming the challenges for AI adoption in engineering processes: Data Management and Model Deployment
- Felix Hildebrand (Robert Bosch GmbH), Hybrid Modeling in Action: Some Challenges and Success Stories at Bosch
- Andras Poppe (BME Budapest) and Susan Zhao (Signify), Towards digital twin based prognostics in LED-based lighting applications
- Henning Sauerland (Hitachi), Nicolo Ripamonti (Hitachi Energy), Integrating SciML into Industrial Applications at Hitachi: Challenges and Opportunities
- Andrea Bonfanti (BMW), Scientific Machine Learning for CFD applied to the automotive use case
- Magnus Fontes (Roche), The Human-Machine Partnership for advancing Biomedicine.
 Learnings and challenges for the future

12.30-13.30 Lunch

13.30-15.00 Round of workshops

The challenges presented by industry in the morning, as well as additional challenges, will be discussed. The findings will be presented and discussed during the dinner.

15.00-15.30 Break

15.30-16.45 Keynote talks

- Victorita Dolean (TU Eindhoven), Parallelization approaches for neural network-based collocation methods
- Yannis Kevrekidis (DARPA), tba
- George Karniadakis (Brown University), Neural operators as foundation models for Digital Twins - ONLINE

16.45-17.30 Panel discussion

<u>Panellists:</u> Sjoerd Verduyn Lunel (ASML), Yannis Kevrekidis (DARPA), Gitta Kutyniok (LMU), Thomas Runkler (Siemens), Magnus Fontes (Roche)

17.30-18.00 Drinks

18.00-21.00 Dinner + discussion of workshop findings

Wednesday, October 16, 2024

09.00-10.25 Keynote talks

- Felix Dietrich (TUM), Learning Hamiltonian dynamics without backpropagation
- Diana Manvelyan (Siemens), Summary of the ECMI Special Interest Group meeting on "Mathematical methods for explainable AI"
- Ling Guo (Shanghai Normal University), *Information Bottleneck based Uncertainty Quantification for Neural Operator Learning ONLINE*

10.25-11.15 Poster pitches

11.15-12.00 Break/poster session

12.00-12.45 Industrial success stories and information on European activities

- Neil Ashton (Amazon Web Services), Large-scale high-fidelity datasets to accelerate ML4CFD progress
- Axel Klawonn (Univ. of Cologne), on the Topical Activity Group Scientific Machine Learning of the European Mathematical Society
- Wil Schilders (TUM-IAS), on the COST proposal for a European network on Scientific Machine Learning

12.45-13.30 Lunch + poster session

13.30-14.30 Discussion of final report for those interested



COST ACTION

The findings in the final report will also be used as input to a proposal for a COST Action that will be submitted soon after the workshop. During the workshop, we will share a link that can be used by participants to support this COST Action.

COST is one of the oldest subsidy programs in Europe, mainly for networking. It stands for "Cooperation in Science and Technology". COST Actions usually have participants from all over Europe, and workshops can be organised during 4 years. COST Actions are a cradle for other collaborative projects, such as MSCA or industry-led projects in ECSEL, ITEA and more.