Fellow	Marius **Kurz**

Host Organisation	Centrum Wiskunde & Informatica (CWI)

Scientific coordinator	Benjamin **Sanderse** Group Leader B.Sanderse@cwi.nl Centrum Wiskunde & Informatica Science Park 123 1098 XG Amsterdam The Netherlands

I – SCIENTIFIC ACTIVITY DURING YOUR FELLOWSHIP

- During my fellowship, I have worked and performed research on turbulence closure modeling using machine learning. In particular, I investigated the use of Graph Neural Networks (GNN) to train machine learning models that comply with the symmetries of the underlying physics. For this, I could rely on the expertise in structure-preserving modeling, machine learning and turbulence in the group *Scientific Computing* at CWI.
- I applied this idea successfully to the task of turbulence modeling for canonical flow cases such as homogeneous isotropic turbulence and turbulent channel flow. The models were trained in actual simulations using Reinforcement Learning (RL) to address the potential mismatch between training a model on precomputed snapshots and dynamic simulations.
- For this research I have continually developed Relexi, which is an open-source reinforcement learning framework for high-performance computing. During my fellowship I extended the framework to SLURM-based systems to run on Snellius, the Dutch national supercomputer and published it as Python package at PyPI to facilitate its use for other researchers in the community.
- Moreover, the GNN models developed in this work were adapted in cooperation with the University of Stuttgart to be applied to the task of active control around a 2D cylinder. Here, the GNNs were used to construct a data-driven control law that is invariant with respect to the ordering of the individual input measurements leading to a model that is more physically consistent and general than the current state-of-the-art.
- I also contributed to a common group project in cooperation with the Deltares research institute to improve the prediction of the failure probability of dikes in the Netherlands. In this project we investigated how elaborate methods from reliability engineering can be used to accelerate the computation of the failure probability considering a range of uncertain influencing factors.
- Besides my active research, I contributed to the scientific community by performing peer review for established, international journals in the field of scientific machine learning, fluid dynamics, turbulence modeling and numerical methods. During my fellowship I conducted peer reviews for the journals:
  - Journal of Computational Physics
  - Physics of Fluids
  - Flow, Turbulence and Combustion
  - Communications Physics
  - European Journal of Mechanics – B/Fluids

II – PUBLICATION(S) DURING YOUR FELLOWSHIP

During the fellowship period at CWI I have published 1 journal article and submitted 2 manuscripts to established international journals:

Kurz, **Marius**, Daniel Kempf, Marcel P. Blind, Patrick Kopper, Philipp Offenhäuser, Anna Schwarz, Spencer Starr, Jens Keim, and Andrea Beck. 2025. "GALÆXI: Solving Complex Compressible Flows with High-Order Discontinuous Galerkin Methods on Accelerator-Based Systems." Computer Physics Communications 306 (January):109388. https://doi.org/10.1016/j.cpc.2024.109388.

(This article was written and submitted prior to the fellowship period, but the revision and publishing process was performed during the fellowship.)

Kurz, **Marius**, Rohan Kaushik, Marcel Blind, Patrick Kopper, Anna Schwarz, Felix Rodach, and Andrea Beck. 2025. "Invariant Control Strategies for Active Flow Control Using Graph Neural Networks." Preprint under review at Computers & Fluids. https://doi.org/10.48550/arXiv.2503.22775.

Kurz, **Marius**, Andrea Beck, and Benjamin Sanderse. 2025. "Harnessing Equivariance: Modeling Turbulence with Graph Neural Networks." Preprint under review at Journal of Computational Physics. https://doi.org/10.48550/arXiv.2504.07741.

III – ATTENDED SEMINARS, WORKHOPS, CONFERENCES

During the fellowship I attended and gave presentations at multiple national and international workshops and conferences:

PASC24 (Platform for Advanced Scientific Computing Conference):
3–5 June 2024 in Zürich, Switzerland.
Title: *Relexi: Reinforcement Learning for Applications in CFD*

3rd AIM Workshop (AI & Mathematics):
13–14 June 2024 in Utrecht, Netherlands.
Title: *Consistent Closure Modeling for Large Eddy Simulation via Reinforcement Learning*

EDFC1 (1st European Fluid Dynamics Conference):
16–20 September 2024 in Aachen, Germany.
Title: *Consistent Turbulence Modeling via Reinforcement Learning*

DUCOMS Day 2024 (Dutch Computational Science Day):
12 November 2025 in Utrecht, Netherlands.
Title: *Equivariant Closure Modeling using Graph Neural Networks & RL*

AICOMAS 2025 (1st ECCOMAS AI and Computational Methods in Applied Science):
17–21 February 2025 in Paris, France.
Title: *Combining Graph Networks and RL for Consistent Turbulence Modeling*

IV – RESEARCH EXCHANGE PROGRAMME (REP)

I visited the Memphis team of Inria Bordeaux in France lead by Angelo Iollo from March 17-21 2025 under the supervision of Tommaso Taddei. During my REP, I presented my research to the team and received an overview of the various field of research conducted in the group. I had several scientific discussions with various members of the group that serve as a basis for potential collaboration and scientific exchange between our groups in the future. Particular points of interest were:

- Encoding physical constraints (in particular symmetries) into the architecture of machine learning models using Graph Neural Networks.
- Using reduced-order models (ROMs) to reduce the computational effort of RL training methods by replacing the costly simulations with a ROM for training.
- Connections between data assimilation and RL, their potential advantages and disadvantages and how either of those methods can be used to achieve long-term stability in ROM inference.
- The suitability of RL and ROMs for tasks in active flow control and challenging turbulent flow cases of particular interest.
- The use of Graph Neural Networks and RL for wall-modeling in large eddy simulation and the current state-of-the-art for this field of application.

V – SUM UP OF THE FINAL SCIENTIFIC REPORT FOR THE ERCIM NEWSLETTER

Marius Kurz' research interests lie in the fields of machine learning, fluid mechanics, and high-performance computing. During his fellowship, he investigated how Graph Neural Networks can be used to embed the rotational symmetries of physical systems into machine learning models. He applied this approach to turbulence modeling and active flow control, resulting in two manuscripts currently under peer review. Following the fellowship, he will join AMD as an application engineer, supporting researchers to run large-scale simulation and AI workloads on modern computing systems.

Learn more or connect with Marius on linkedin.com/in/m-kurz/.