Project: **1372**
Project title: **ExaOcean**
Principal investigator: **Maximilian Witte**
Report period: **2024-05-01 to 2025-04-30**
Maximum of 2 pages including figures. 9 pt minimum font size.

Allocations 7/2024 to 6/2025

Resource	Granted	Utilization	Remaining
Levante CPU nodes (Node hours)	1000	751	249
Levante GPU nodes (Node hours)	7500	6426	1074
Levante storage (TiB)	100	64	36
Archive project (TiB)	50		50
Archive long term (TiB)	10		10
Swift Object Storage (GiB)	10240		10240

Figure 1: Allocated and used ressources (29.04.25).

Justification of expired resources (Figure 1)

Resources were expired mostly due to development phases of the ML models on local machines. In this project we generally try to carefully test our ML models, which are mostly written from scratch, before we enter large scale trainings.
As a result, some resources may expire, when development/testing takes longer than expected. In December 2024, some resources expired due to sickness and holiday.

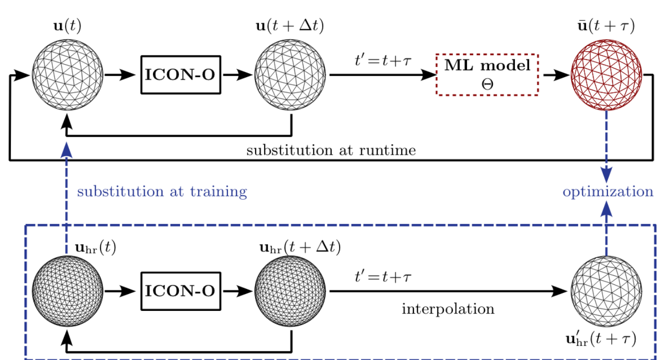

Figure 2: Published hybrid approach combining numerical simulation using the ICON-O model with machine learning based super-resolution (SR-ICON) [1]. The data flow during runtime is indicated by the solid arrows (top panel), while the dashed blue lines indicate the data flow during training. Δt is the time step used in the numerical simulation (ICON-O). At t = 0 and τ ≫ Δt, we use a distance-weighted interpolation method (CDO) to map the high-resolution ground truth of the simulation onto the low-resolution grid for the input and the ground truth of the ML model Θ training [1].

Results of ExaOcean

The main, hybrid approach introduced in the first period of ExaOcean is shown in Figure 2.
The ML model is trained to learn the difference between the low- and high-resolution simulations at each τ. For the chosen test-case (Galewsky, shallow water), τ was chosen as $\tau = 12h$. At runtime, the ML model corrects the low-resolution data. See [1] for more details.

In the subsequent stage (last period, 06/2024-07/2025) we switched to the full ocean (3D) using the baroclinic test case [2]. We used ocean channel-data in terms of a patch with 500m resolution and periodic longitudinal boundary conditions.

To make the model learn different dynamics across the depth of the ocean, we introduce a depth embedding, which is added to each layer of the UNet model Θ, which is used as a core. The depth embedding is shown in figure 3.

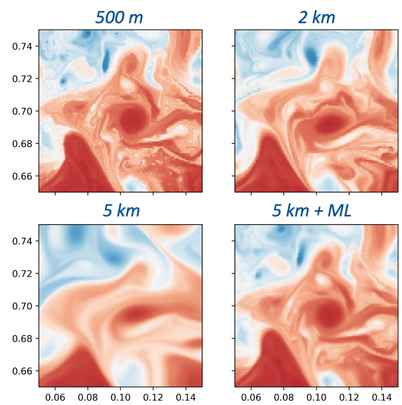

Figure 3: Snapshots of surface temperature integration of the 3D Ocean of the baroclinic instability of the 20th day of the validation data set. Top left: Reference on a 500m grid. Snapshot of surface temperature integration of our SR-ICON-O approach (bottom right) for the 3D Ocean of the baroclinic instability of the 20th day of the validation data set.

Development of a Transformer model based on the ICON grid

Another branch of the project is the replacement of the Unet with a Multi-Grid Transformer model defined on the ICON grid. As a first benchmark, we compare our model against the Unet in a downscaling experiment of Era5 data from 550km (17x) back to the resolution of Era5. In total, our model outperformed the Unet. It slightly consumes more memory than the Unet, leading to higher training and inference times. Compared to other large-scale models, the computational performance seems to be still quite low (needs verification). Introducing variable constraints by factorizing the weight matrix increases the speed of convergence [3].

We will investigate the use of our transformer model (Figure 4) in our hybrid modelling approach.

[1] Maximilian Witte et al 2025 Mach. Learn.: Sci. Technol. 6 015060
[2] Salmon, Rick. "Baroclinic instability and geostrophic turbulence." *Geophysical & Astrophysical Fluid Dynamics* 15.1 (1980): 167-211.
[3] Kossaifi et al., 2024. Multi-Grid Tensorized Fourier Neural Operator for High- Resolution PDEs