# Innovative Computational Science by Integration of Simulation/Data/Learning on Heterogeneous Supercomputers

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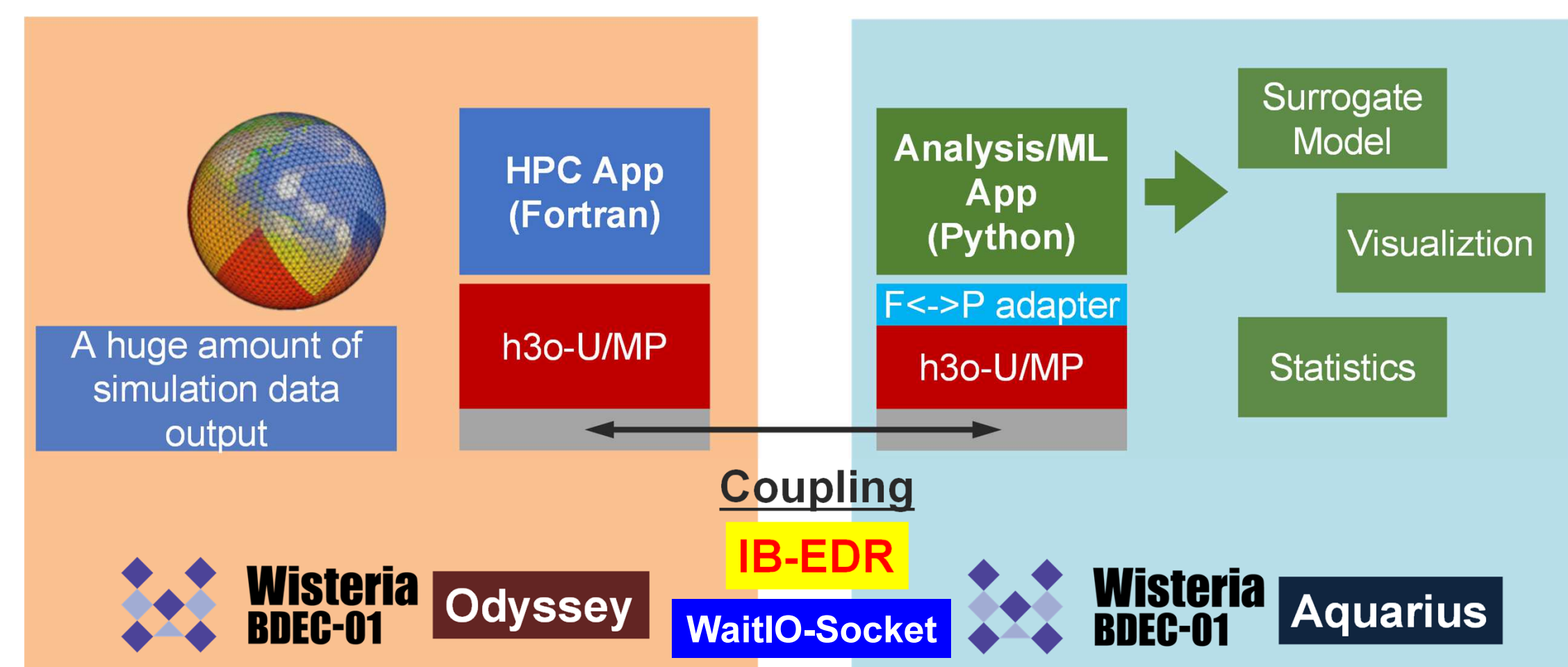
Overview

- This project advances computational science by integrating "Simulation/Data/Learning (S+D+L)" using heterogeneous supercomputers such as "Wisteria/BDEC-01 (U.Tokyo)" and "Miyabi (JCAHPC)", along with "mdx."
- While our focus was earthquake simulation with real-time data assimilation in FY.2021/2022, we expand the "S+D+L" concept to other fields, initiating joint research and software development with international partners in FY.2023.
- Most of the members have been working on the innovative software platform "h3-Open-BDEC since FY.2019 to facilitate "S+D+L" integration on heterogeneous systems.
- Wisteria/BDEC-01 ("Odyssey" for Simulations with A64FX, "Aquarius" for Data/ML/AI with NVIDIA A100) operates as a full-scale platform for "S+D+L" integration with h3-Open-BDEC, gaining global attention.
- In FY.2023 and FY.2024, we have conducted research in earth science, life science, and library/software/tool for integration of "S+D+L".
- In FY.2025, we add a new field (quantum sciences), and extend the idea of h3-Open-BDEC for QC (Quantum Computers)-HPC Hybrid Environment.
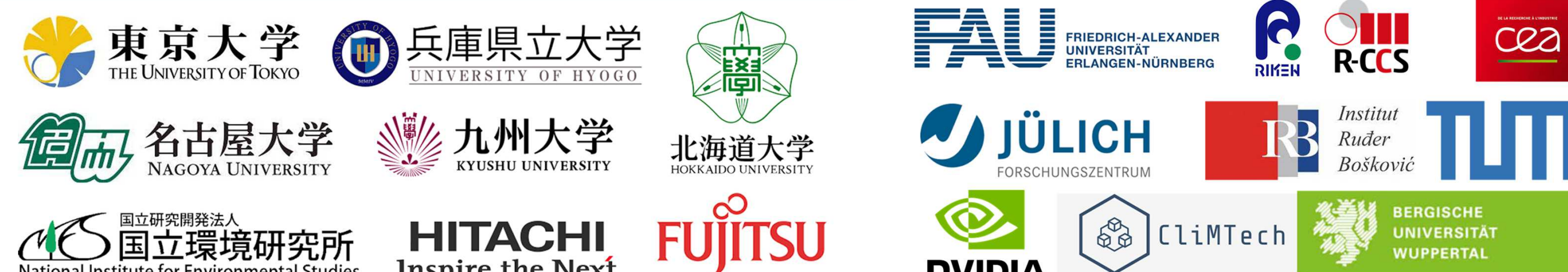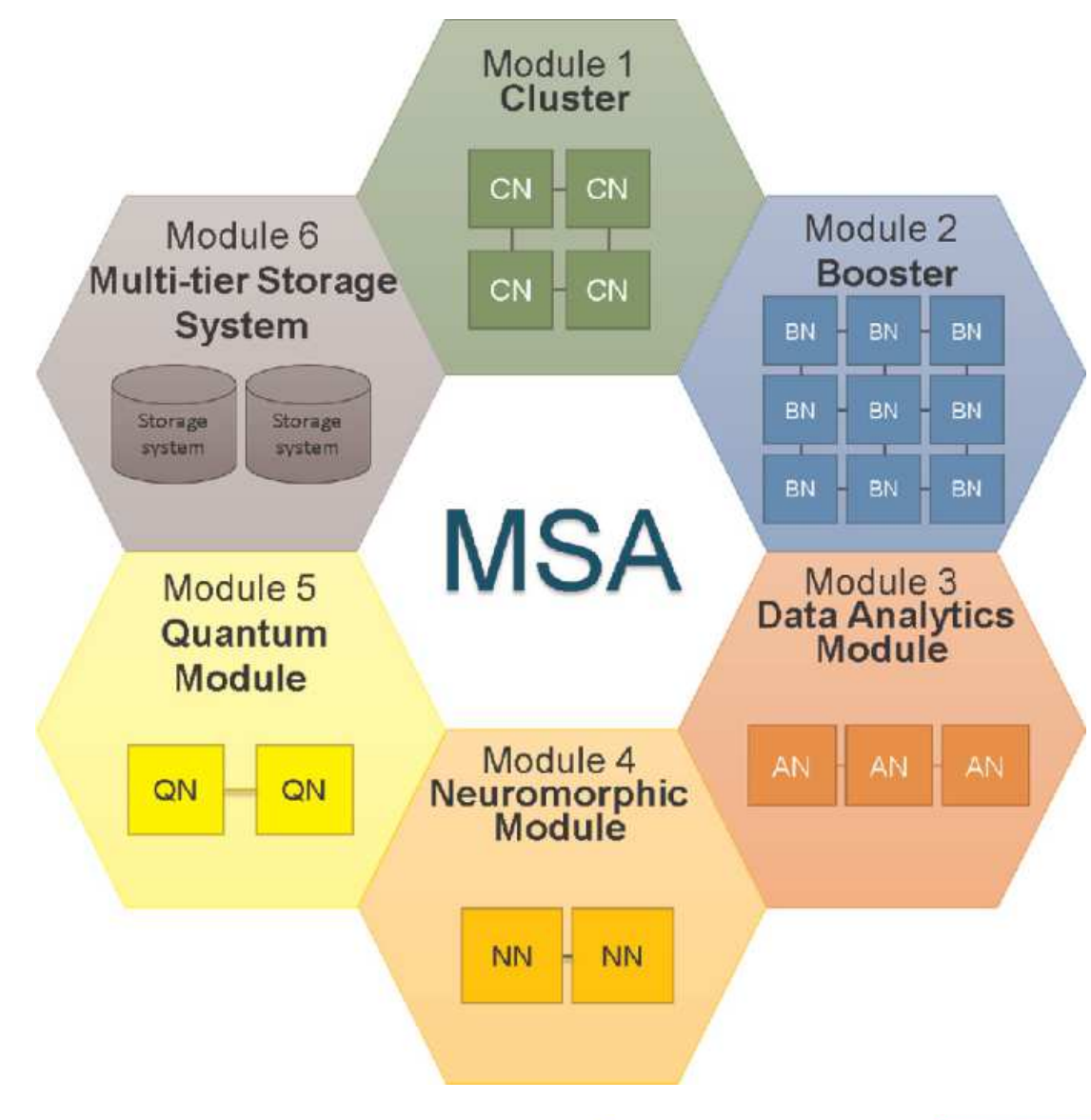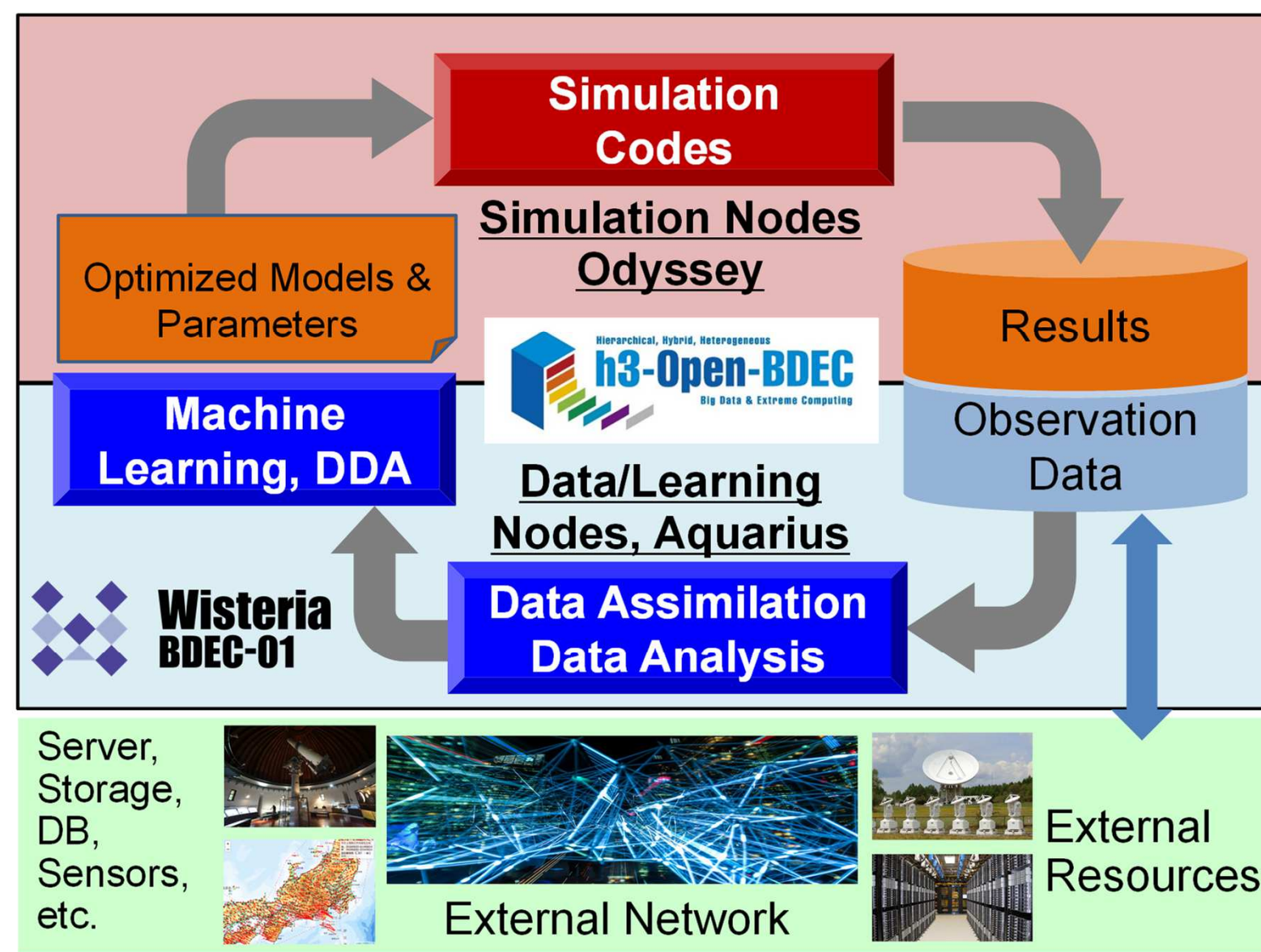
Integration of (S+D+I) by h3-Open-BDEC: WaitIO-Socket and Coupler (h3o-U/MP)
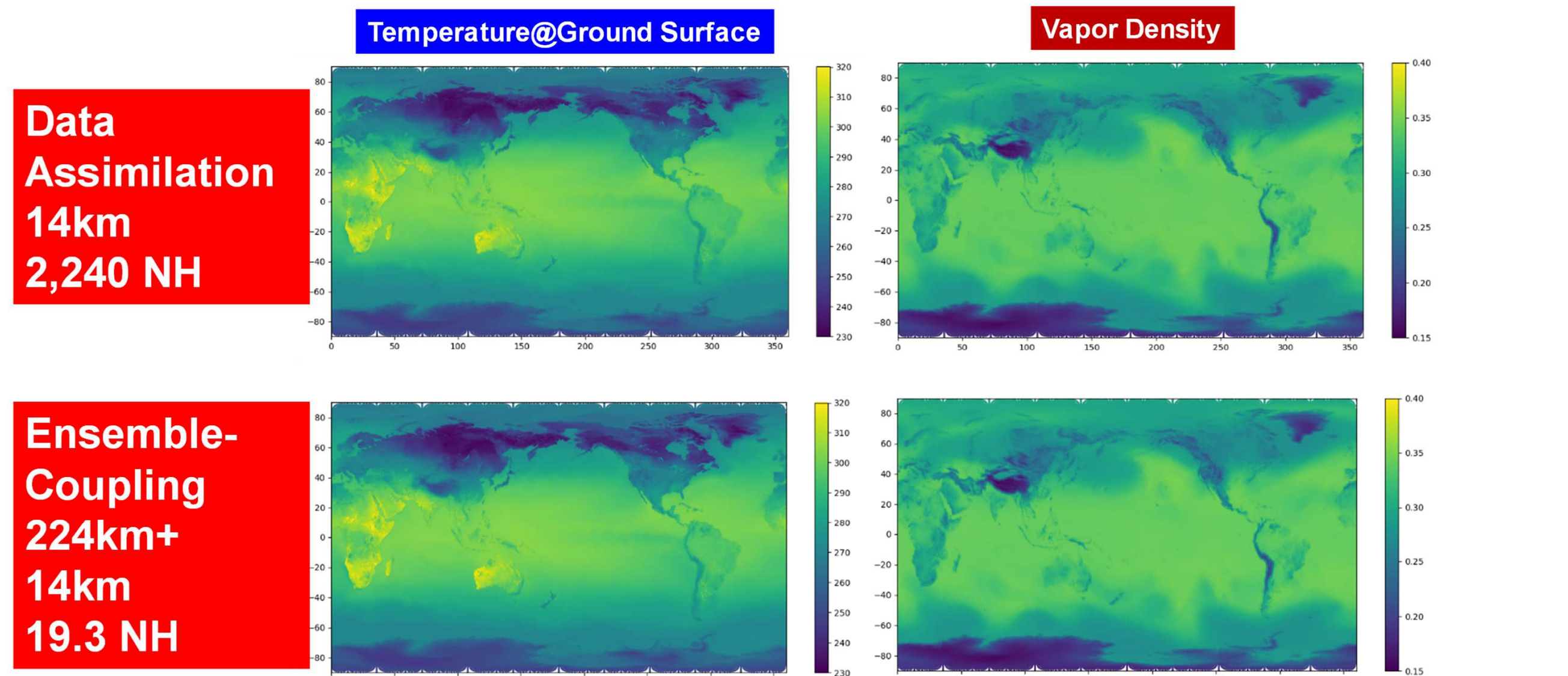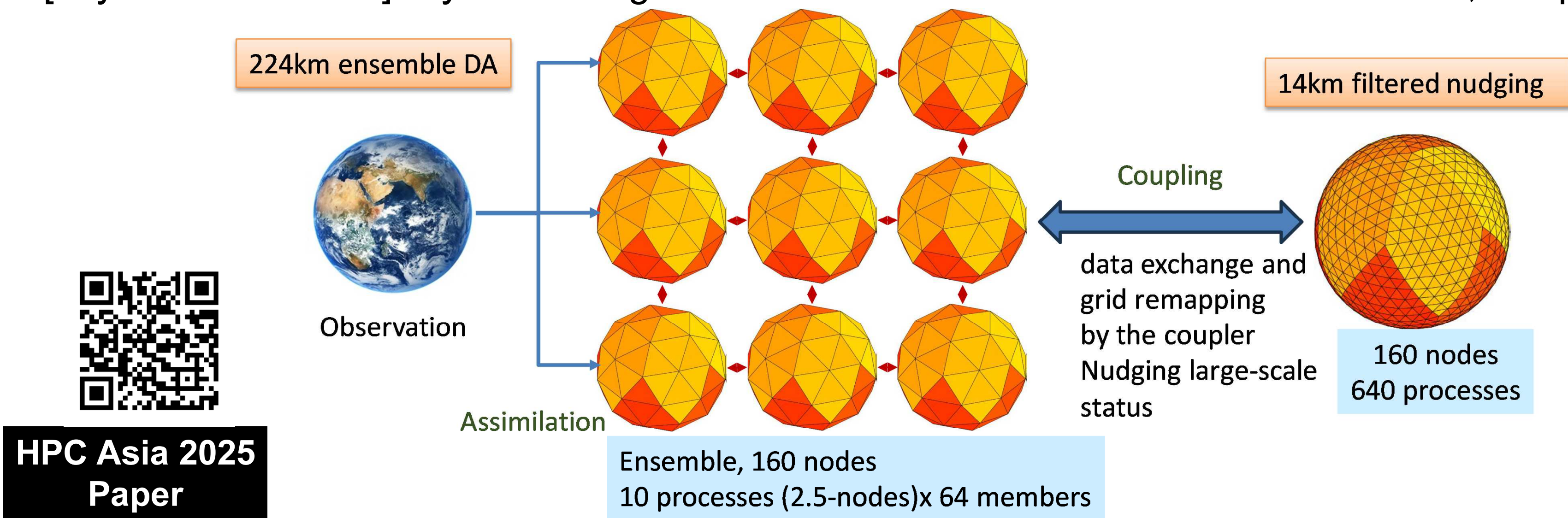
- h3-Open-SYS/WaitIO-Socket (WaitIO-Socket) is a system-wide communication library to couple multiple MPI programs for heterogeneous environments, such as Wisteria/BDEC-01, which provides an MPI like API and can easily connect multiple MPI programs.
- h3-Open-UTIL/MP (h3o-U/MP) originally provides capabilities for multi-physics coupling between different grid systems. Furthermore, it is equipped with a function for combined ensemble, and with an interface for coupling codes for large-scale simulations on Odyssey and ML/AI applications written in Python on Aquarius
  - While such coupled computing has been only possible by MPI on a single/homogeneous system, h3o-U/MP with WaitIO-Socket provides more flexible interface for integration of (S+D+L) on heterogeneous system, such as Wisteria/BDEC-01.
- **In this project, we apply h3-Open-BDEC to various types of workloads by partners' codes towards integrations of (S+D+L)**

Ensemble Coupling for Global Atmospheric Simulations

- We improved the h3o-U/MP to enable **ensemble coupling** of low-resolution (224 km mesh) ensemble simulations and high-resolution model (14 km) simulations for global atmospheric simulations.
- **A simulation including a low-resolution ensemble of 64 cases was performed in FP32 using 320 nodes of Wisteria/BDEC-01 (Odyssey), and the results were compared with a high-resolution ensemble of 64 cases in FP64. In a trial simulation for 9 hours, we achieved approximately 100 times the computational efficiency while maintaining accuracy (2,240 node hours ⇒ 19.3 node hours).**
- **The paper on this issue was presented in HPC Asia 2025 conference.**
- In weather forecasting, the number of ensembles for data assimilation is approximately 50-100 due to limitations in computational resources and time in current medium- to long-term forecasts, but it is known that highly accurate forecasts can be made by performing data assimilation of approximately 1,000 ensembles. [Miyoshi et al. 2014]. By increasing the number of ensembles at a lower resolution, it is possible to issue more accurate forecasts with the same calculation time.


HPC Asia 2025 Paper

224km ensemble DA — Observation — Assimilation

Ensemble, 160 nodes
10 processes (2.5-nodes)x 64 members

Coupling
data exchange and grid remapping by the coupler
Nudging large-scale status

14km filtered nudging
160 nodes
640 processes

Temperature@Ground Surface / Vapor Density

Data Assimilation 14km 2,240 NH

Ensemble-Coupling 224km+ 14km 19.3 NH

(Part of) Target Applications in FY.2025

Terrestrial Systems Modeling Platform (TSMP)

- TSMP is a scale-consistent, highly modular, massively parallel, fully integrated soil-vegetation-atmosphere modeling system by JSC.
- Our target is coupling COSMO/ICON (Atmosphere)-ParFlow (Surface/Subsurface Flow)-CLM(Land Surface Model).
  - The coupling of 3 models has been already done using OASIS3 library on CPU-GPU heterogeneous environment of DEEP System in JSC based on MSA
- **In FY. 2024, we have replaced OASIS3 with h3-Open-BDEC. on Wisteria/BDEC-01 and DEEP.**
  - **Joint Paper was presented at AGCA WS in conjunction with PPAM 2024**
- **In FY.2025, we plan to do full coupled simulation of TSMP using h3-Open-BDEC on Wisteria/BDEC-01 and Miyabi.**
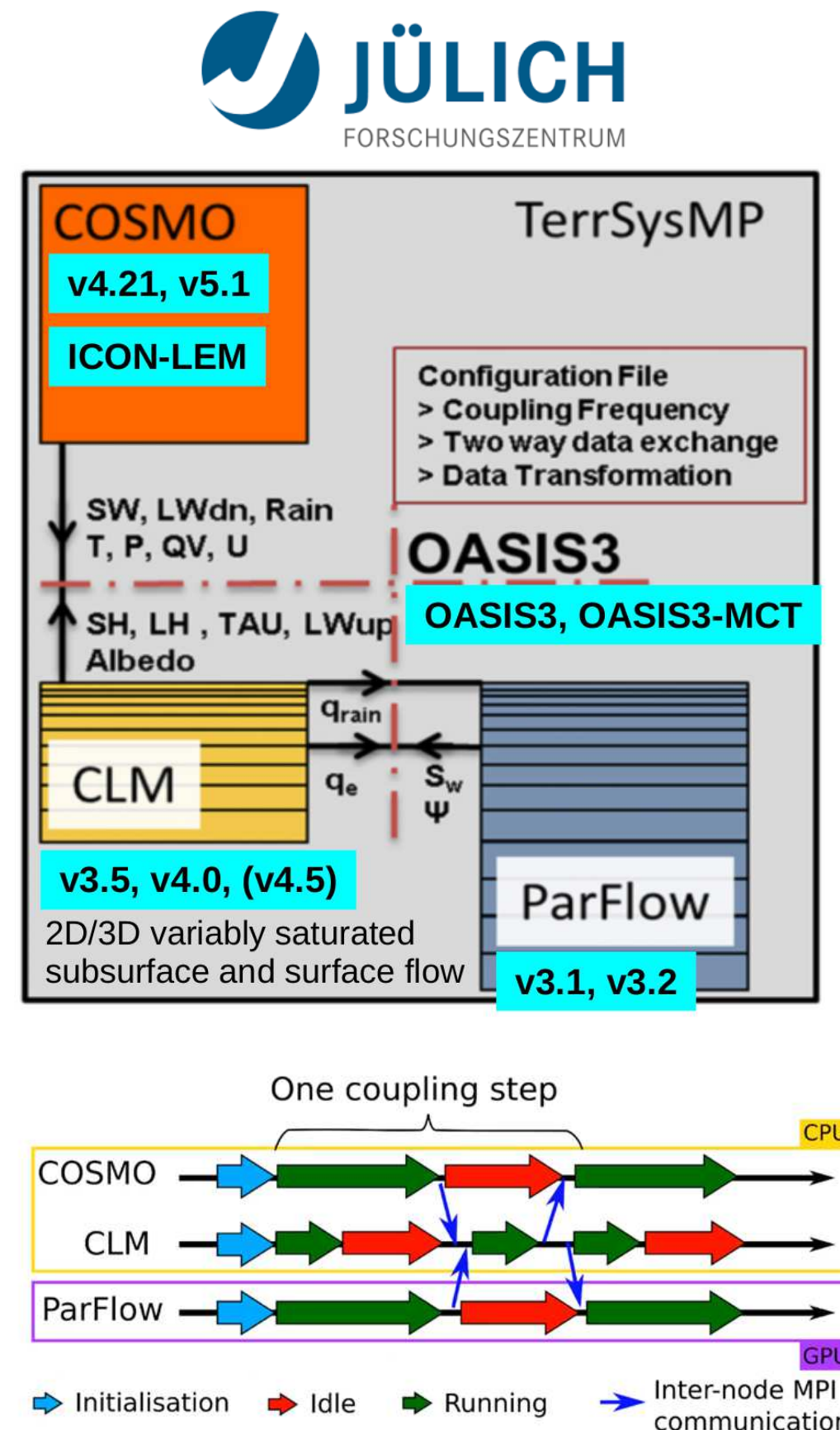
Quantum-HPC Hybrid Environment

- In JHPC-quantum project, h3-Open-BDEC is utilized for development of hybrid environment with Quantum Computers (QC) and Supercomputers (HPC).
- A "pseudo" QC-HPC Hybrid Environment on Wisteria/BDEC-01, utilizing Aquarius with NVIDIA's CUDA-Q (https://developer.nvidia.com/cuda-q) as QC and Odyssey as HPC.
  - Simple VQE (variational quantum eigensolver) with 4 qubits
- Next Step
  - 20+ qubits
  - QC-HPC Hybrid Subspace Method based on QSCI for quantum chemistry, leveraging QC for subspace projection and HPC for diagonalization.

TSMP Terrestrial Systems Modeling Platform

AGCA/PPAM 2024 Paper

Wisteria BDEC-01