HANAMI

# HPC ALLIANCE FOR APPLICATIONS AND SUPERCOMPUTING INNOVATION: THE EUROPE – JAPAN COLLABORATION

Funded by the European Union

EuroHPC Joint Undertaking

This project received funding from the European High Performance Computing Joint Undertaking (EuroHPC JU) under the European Union's Horizon Europe framework program for research and innovation and Grant Agreement No.101136269. Views and opinions expressed are, however, those of the author(s) only and do not necessarily reflect those of the European Union or EuroHPC Joint Undertaking. Neither the European Union nor the granting authority can be held responsible for them.

# DELIVERABLE 1.7

## Follow-up of the scientific collaborations with Japanese partners - 2

| | |
|---|---|
| **Project Title** | Hpc AlliaNce for Applications and supercoMputing Innovation: the Europe - Japan collaboration |
| **Project Acronym** | EuroHPC International Cooperation (HORIZON-EUROHPC-JU-2022-INCO-04) |
| **Project Number** | HANAMI |
| **Type of Action** | 101139786 |
| **Topic** | HORIZON JU Research and Innovation Actions |
| **Starting Date of Project** | HORIZON JU Research and Innovation Actions |
| **Ending Date of Project** | 2024-03-01 |
| **Duration of the Project** | 2028-02-28 |
| **Website** | 36 months |

| | |
|---|---|
| **Work Package** | 1 |
| **Task** | 1.7 |
| **Lead Authors** | France Boillod-Cerneux (CEA) , Edouard Audit (CEA) |
| **Contributors** | All members of HANAMI |
| **Peer Reviewers** | Erik Lindahl (KTH), Joachim Biercamp (DKRZ), Christophe Calvin (CEA) |
| **Version** | 3.0 |
| **Due Date** | 28.02.25 |
| **Submission Date** | 27.02.25 |
| **Re-submission Date** | 08.12.25 |

## Dissemination Level

| | |
|---|---|
| X | PU: Public |
| | SEN: Sensitive – limited under the conditions of the Grant Agreement |
| | EU-RES. Classified Information: RESTREINT UE (Commission Decision 2005/444/EC) |
| | EU-CON. Classified Information: CONFIDENTIEL UE (Commission Decision 2005/444/EC) |
| | EU-SEC. Classified Information: SECRET UE (Commission Decision 2005/444/EC) |

## Disclaimer

Funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or EuroHPC Joint Undertaking. Neither the European Union nor the granting authority can be held responsible for them.

# Version History

| Revision | Date | Editors | Comments |
|---|---|---|---|
| 1.0 | 01.02.25 | France Boillod-Cerneux (CEA) | Template to retrieve the HANAMI work packages information. |
| 1.1 | 15.02.25 | HANAMI members | Providing inputs for all work packages |
| 2.0 | 27.02.25 | France Boillod-Cerneux (CEA) | Gathering the work packages presentations and consolidating the deliverable. |
| 3.0 | 08/12/25 | France Boillod-Cerneux and christophe calvin (CEA) | Modifications requested by RM18 |

# Executive Summary

This deliverable focuses on the follow-up of HANAMI collaboration with Japanese partners.
In the following presentation, we present HANAMI work packages in strong interaction with HANAMI Japanese partners and details ongoing and future actions, designed and led jointly by European and Japanese researchers involved within HANAMI.
This document will serve as a basis to highlight HANAMI collaboration with Japan, and will be regularly updated, leading to respectively D1.8, D1.9 and D1.10.
For more details about each scientific project, we invite the reader to consult the deliverables written by WP4, WP5 and WP6 respectively.

# Table of Contents

# 1. WP4 - Application development for the climate and weather modelling community

The WP4 connects Japanese and European efforts and expertise to improve the performance of codes for weather and climate simulations. WP4 has the following objectives:

- Assess and improve the computational performance, replicability and accuracy of our European Earth System Models as a whole, tested on European and Japanese HPC platforms
- Optimize, port and test European models on Japanese supercomputers
- Incorporate Japanese weather and climate codes into our European benchmarks to be used on EuroHPC platforms

We provide below a follow up of the activities between European and Japanese researchers for each project of the WP4.

## Project 1: Replicability and skill of earth system models - Workflow and Interface

| | |
|---|---|
| Objectives | **Task 4.1: Model assessment for earth system models and the integration through the workflow manager Autosubmit**<br>Partners: BSC, DKRZ, RCCS, NIES<br>The researchers develop a workflow (orchestrator and monitor in a self-contained application) for testing three aspects of earth system models (ESM): 1. replicability, 2. projection skill, and 3. computational performance. HANAMI combines those methodologies inside a single workflow with a generic interface applicable to any weather and climate model and accessible on any cluster. |
| Working process and collaboration format | HANAMI has deployed the new workflow on European and Japanese supercomputers and developed a strong collaboration connecting Japanese and European efforts on weather and climate model development. HANAMI has set up a collaborative effort for the future in porting European and Japanese models to the workflow and assessing their replicability, projection skill, and performance on European and Japanese supercomputers.<br><br>Visits and exchanges:<br>• Planning a long stay of Marta Alerany at JAMSTEC in May (6 weeks): Marta Alerany and Kai Keller will attend the JpGU meeting in May in Tokyo (session on high resolution modelling, convener: Hisashi Yashiro)<br>• First travel and internship in October 2024 successfully completed: Leo Arriola stayed at NIES for a 5 weeks internship. Leo gave a talk at the University of Tokyo, presenting HANAMI and the HANAMI workflow. Leo Arriola & Kai Keller visited the 10th International Symposium on Data Assimilation (ISDA), Met in |

| | |
|---|---|
| | person with Chihiro Kodama and Hisashi Yashiro at NIES, Mohamed Wahib (RIKEN)<br><br>Regarding codes and applications:<br>The model NICAM coupled to COCO (NICOCO) was ported to Marenostrum5 and Fugaku. The HANAMI Autosubmit workflow was developed which compiles the model and runs simulations on both platforms (Joint workflow development for NICOCO in Autosubmit). EC-Earth has been compiled on Fugaku and Marenostrum5.<br><br>For more details about these results, we invite the reader to consult the technical report and D4.1. |
| Leverage actions | The researchers have submitted 1 joint proposal to the JHPCN international project<br>• Miyabi access track<br>• Travel and conference funding<br>• This proposal is submitted by our Japanese partners but have been codesigned with the HANAMI researchers. |
| Supercomputers acces | The researchers have submitted the following joint proposals to get access to supercomputers:<br>○ Fugaku general access (rejected, in the top 20%, resubmission in May for October access)<br>○ Access granted for WP4P1 European team to Fugaku through HPCI access – duration: 05.2024 until 04.2025, Maximum of computing hours: 40000 Nh<br>○ Development access on Marenostrum5 - duration: 10.2024 until 09.2025, Maximum computing hours (node hours): 4000<br>○ Access granted for WP4P1 Japanese researchers to LUMI through bilateral MoU CSC and RIKEN/R-CCS – duration: 05.2024 until 04.2026, Maximum of computing hours: 40000 |
| Future plans | The team is working on combining the methodologies (replicability, projection skills and computational performance) to propose a single workflow with a generic interface applicable to any weather and climate model and accessible on any cluster.<br>The team is also planning new visits and exchanges to strengthen the EU/Japan collaboration. |

## Project 2: Optimize, port and test European and Japan weather and climate codes

| | |
|---|---|
| Objectives | **Task 4.2: High-Performance Climate and Weather benchmark**<br>DKRZ, BSC, ECMWF, CSC, NICAM<br>○ Extending the existing test cases in HPCW; assistance with implementation of NICAM-DC into HPCW; general maintenance and preparations for first open-source release of HPCW<br>○ Preparing HPCW for MN5 deployment<br>○ Worked on extending NICAM-DC benchmark in HPCW to higher resolution test cases, began investigation of integrating Japanese SCALE model in to HPCW to complement NICAM-DC<br>○ Began building of and preparations for running the HPCW codes on LUMI |
| Working process and collaboration format | Monthly WP4-wide meetings (including Japanese partners): Coordination with Japanese partners on Japanese HPCW components (such as the NICAM code) |
| Supercomputers acces | Access granted to Fugaku for HPCW porting via Fugaku Trial Access – duration: 02.25 until 08.25. Maximum of computing hours: 50000 Nh |
| Future plans | HANAMI members have requested travelling grants within HANAMI (on 06.2024).<br>The following visits are planned:<br>• 2-4 weeks trip to Hisashi Yashiro, NIES (Tsukuba, Japan) for Samuel Hatfield and Niclas Schroeter under discussion, to take place in January 2025<br>HANAMI publications and presentations at international conferences:<br>• Joint session proposal at JpGU, May 2025, under discussion with Hirofumi Tomita (R-CCS), Hisashi Yashiro (NIES), and Chihiro Kodama (JAMSTEC) (1 week trip to Japan for WP4 leaders) |

**Task 4.3: The University of Warsaw Lagrangian Cloud Model (UWLCM) (effective work starts in M19)**

| UW, RIKEN | |
|---|---|
| Objectives | ○ Optimize UWLCM code for modern European and Japanese computing clusters and to deploy it there. In UWLCM, computations can be done on CPUs only or simultaneously on CPUs and on GPUs. So far, scalability has been tested only in the CPU+GPU mode for up to 40 nodes. We propose to test scalability on larger heterogeneous clusters, preferably on LUMI. To achieve this, we will need to adapt the code for AMD GPUs, as it can currently run only on NVIDIA GPUs<br>○ Test and optimize scalability of the CPU-only mode on large CPU-only clusters, such as the Fugaku at RIKEN. We have been collaborating with Dr. Shin-ichiro Shima from the University of Hyogo, who uses Fugaku to run a LES model called SCALE-SDM. Recently, his group has shown that optimizing cache usage can greatly increase performance of Lagrangian microphysics. Within the proposal, we plan to explore the possibility of using similar optimizations in UWLCM |

| | |
|---|---|
| Working process and collaboration format | The researchers have established interactions with WP4 members during online meetings and with the entire Hanami team during High Level Symposium 1.<br>The HANAMI researchers also have monthly meetings with Japanese researchers<br>• Regular exchanges on ICON, and exchanges and information on the UWLCM framework<br><br>More details regarding the results and outcomes are given in D4.1. |
| Supercomputers acces | The researchers have asked for LUMI and FUGAKU access via the Hanami call. |
| Future plans | The effective work is scheduled to start in the second part of 2025 (M19).<br>The researcher has asked for HANAMI travelling grant requested on 07.2024, for 2 weeks duration:<br>• Visit from researchers planned in 2025/2026<br>• Visited laboratory: University of Hyogo, Kobe, Japan |

# 2. WP5 Biomedical application co-development to address societal challenges

The WP5 connects Japanese and European efforts and expertise to improve the performance of codes for biomedical area. WP5 has the following objectives:

- Advancing molecular life sciences computing by joint development of Exascale-focused algorithms
- Pursing data-driven life science by developing new HPC models to integrate experimental data such as cryoEM/ET, single-molecule FRET and high-speed AFM in molecular modelling and simulations.
- Developing techniques to perform whole-minimal-cell simulations with hundreds of millions of coarse-grained particles.
- Developing a comprehensive pipeline for cancer genome analysis in the context of the International Cancer Genome Consortium and European 1+ million genomes based on recommendations and network of standards in the Global Alliance for Genomic Health.
- Implementing a pipeline for simulation of tumour evolution based on individual genomic information within the PhysiBOSS cell-scale simulation environment.
- Combining large-scale computational fluid dynamics simulations with machine learning techniques for an improved analysis of respiratory diseases and virus particle spread in indoor scenarios

We provide below a follow up of the activities between European and Japanese researchers for each project of the WP5.

## Project 1: Exascale electrostatics & machine learning to enable molecular dynamics of cell-size systems

This project extends existing collaborations on software and hardware in molecular dynamics simulation into long-term coordinated development of the two major-impact codes GROMACS (EU) and GENESIS (RIKEN). The project 1 manages the coordination with the simulation hardware developed in the RIKEN MD-GRAPE project. The two codebases GENESIS and GROMACS complement each other: both codes used as benchmarks and optimization targets in the post-Fugaku projects, which leads to a unique codesign opportunity for both the European and Japanese researchers.

| | |
|---|---|
| Objectives | **T5.1: ExaFMM - solving the scaling problem for electrostatic interactions**<br>KTH, R-CCS, The Tokyo institute of technology<br>○ Explore FMM to enable both GROMACS and GENESIS to scale to hundreds of thousands of ranks |

| | |
|---|---|
| | ○ combine the world-leading EU-based molecular simulation code GROMACS with the world leading FFM package ExaFMM developed by Rio Yokota. Turns ExaFMM into a library that can be coupled efficiently to GROMACS Integrate the same code with GENESIS<br>○ Enable both longer simulation times for a given system size, as well as the ability to simulate extreme-scale systems such as entire cells with hundreds of millions of particles.<br><br>**T5.2 - Data-driven biomolecular modelling & simulation**<br>KTH, R-CCS, RIKEN BDR, University of Groningen, Nagoya University<br>○ work on improving the support for neural network/deep learning potentials by integrating DeepMD and other packages into both GROMACS and GENESIS, Evaluate the possibility of directly implementing code to do the inference stage<br>○ Address the challenges with sensitivity to training domains, investigate possibilities to use “delta-learning”, Apply neural networks as a correction<br>○ Develop new algorithms to combine this type of data, develop code to make it possible to restrain an ensemble of simulations, Extend GROMACS to make it possible to perform coarse-grained molecular modelling of cell scale systems restrained with low-resolution experimental data |
| Working process and collaboration format | Active collaboration with Japanese researchers regarding Long-range electrostatics work<br>• Online meetings are held to share updates and coordinate efforts<br>• Extensive RIKEN contributions to GROMACS SVE acceleration and regression testing on Fugaku hardware<br>• Joint Exascale-target fast multipole implementation is actively ongoing with Prof. Rio Yokota (A shared repository is hosting code compatible with both GROMACS and ExaFMM)<br>• A joint publication is planned for the ongoing work related to the regularized fast multipole method<br>• An interface between ExaFMM and GROMACS has been implemented and is ready for integration into GROMACS<br>• RIKEN-CCS GENESIS team is involved in definitions of joint file formats and data exchange standards run by the EU teams |
| Future plans | Planned research visits:<br>• Dr. Muhammad Sadiq to visit Tokyo Tech mid-to-late 2025 for joint ExaFMM work<br>• Prof. Berk Hess visit to RIKEN & Tokyo Tech planned mid-to-late 2025 to finalize work<br>• Prof. Erik Lindahl to visit RIKEN-CCS & RIKEN-BDR in Kobe both 2025 & 2026 to work on data-driven simulations and applications to large systems<br><br>New AI4SCIENCE frameworks both in Sweden & Japan to focus on data-driven work and foundation models. HANAMI will pursue new collaborations with Profs. Yuji Sugita & Satoshi Matsuoka. |

## Project 2: Development of genome analysis pipelines for Personalized Medicine

This project provides mechanistic models for individual patients reflecting their differential genomic composition and response to treatments. Project 2 interprets mechanistic models with field-experts to identify potential treatments and/or associated signatures. The project also contributes to the technical development of practical implementations that facilitate the work of clinicians and genome scientists, ultimately leading to better and more tailored treatment strategies for cancer patients.

| | |
|---|---|
| Objectives | **T5.3: Genome analysis pipeline**<br>BSC, CSC, The university of Tokyo, Osaka University<br>○ genome analysis pipeline with variants for different type of genomic data<br>○ use different type of genomic and clinical information including real data complemented with generated synthetic data<br>○ modelling of the cohorts of synthetic data between the participating labs in Japan and Europe<br>○ data sets analysed in the context of the information available in large cancer projects and repositories, including ICGC and others sources of genomic data at the single cell level, e.g., tissue specific single cell expression data recently published.<br><br>**T5.4 - Tumour evolution simulation pipelines**<br>BSC, CSC, The university of Tokyo, Osaka University<br>○ Adaptation of the intracellular pathways to the patient specific data (mutations and gene expression levels) and the simulation of tumour evolution within the PhysiBoSS agent-based component.<br>○ integration of the genome analysis and simulation workflows and their adaptation to the operation in new hardware environments, with particular emphasis in new implementation adapted to GPU infrastructures<br>○ produce pipelines that can be executed by non-experts without the need of further adaptations beside setting the input data and basic parameters |
| Working process and collaboration format | Monthly meetings with Japanese researchers to evaluate synthetic data generation pipelines: How to integrate somatic alterations from real patients to improve synthetic data quality and potential applications in Personalised Medicine and computational biology<br><br>Monthly meetings with Japanese researchers to identify grand challenges in Personalised Medicine requiring exascale capacities<br>• Large-scale prediction of combinatorial drug treatments<br>• Explore landscape of attractors in super complex molecular pathways<br>• Integration of genome-scale metabolic networks in cellular simulations<br>• Hero runs: From molecular features to whole organ simulations<br><br>Coordinate efforts for computationally benchmarking of genomic pipelines on European and Japanese HPC facilities |

| | |
|---|---|
| | • Comparative test in MN5-LUMI vs Fugaku: Evaluate parallel and distributed computing efficiency on synthetic data generation pipelines and tumour evolution multiscale simulations |
| Future plans | Plan researcher visits in Japan<br>Co- organise workshops on HPC-simulations in biology<br>Explore opportunities for joint publications |

## Project 3: Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses

Project 3 aims to develop a pipeline for AI-assisted, automated large-scale CFD simulations to analyse respiratory diseases. Project 3 uses advanced AI methods to accelerate these simulations. As part of this effort, project 3 also provides surgeons with an AI-assisted automated surgery tool as a demonstrator and create a tool for assessing the risk of exhaled infectious viruses in indoor scenarios. All implementations are designed to complement missing elements in either the m-AIA (EU) or the CUBE (Japan) CFD solvers. Within project 3, the AI methods are being jointly developed with our Japanese partners.

| | |
|---|---|
| Objectives | **T5.5: AI-assisted automated CFD pipelines and acceleration of CFD computations**<br>FZJ, RIKEN Kobe University<br>○ Accelerating 2D and 3D CFD simulations by flow field initialization with a meaningful approximation coming from physics-aware convolutional neural networks: 2D flow through a randomly constricted channel, 2D flow around random shapes, 3D flows through a randomly constricted 90-degree elbow pipe<br>○ Predicting 2D flow fields by physics-aware graph convolutional neural networks: 2D flow through a randomly constricted channel, 2D flow around random shapes, Training physics-informed neural networks for flow predictions based on sparse spatial and temporal data<br>○ Employing deep learning techniques for flow field decomposition to investigate different modes of flow fields<br><br>**T5.6 - AI-assisted surgery planning and risk assessment of exhaled infectious aerosols**<br>FZJ, RIKEN Kobe University<br>○ Improving the efficiency of the surgery planning tool by coupling the reinforcement learning algorithm with a gaussian process regression model, training a graph convolutional neural network to predict nasal cavity flows for an acceleration of the feedback loop in the reinforcement learning algorithm<br>○ Coupling of m-AIA with reinforcement learning environments for 3D benchmark problems: controlling surface jets to reduce drag for 3D flow around a cylinder and 3D flow around a sphere<br>○ Coupling CUBE simulations of indoor scenarios to a genetic algorithm to optimize the interior design of clinical facilities |

| | |
|---|---|
| Working process and collaboration format | Monthly meetings with Japanese researchers to exchange progress of the Joint Laboratory for Extreme Scale Computing (JLESC) Project "Deep Neural Networks for CFD Simulations"<br>Further online meetings to achieve the following:<br>• Joint publication about physics-informed neural networks for flow predictions<br>• Joint publication about the decomposition of flow fields with machine learning<br>• Joint submissions to the Workshop on Advancements of Global Challenges Applications (AGCA), held in conjunction with the 15th International Conference on Parallel Processing and Applied Mathematics PPAM 2024<br>• Recent publication on experimental-data-driven boundary conditions for LBM simulations - this application can be extended for boundary conditions for respiratory flow simulations<br>• Another paper is currently in review to advance the use of CFD in rhinology<br><br>FZJ also participates in AI4HPC project, which provides a repository of useful AI models trained on CFD datasets. This repository can also be used as a shared workspace to integrate the models and datasets generated by the Japanese researchers at RIKEN-CCS and Kobe University. They can also have unrestricted access to models and datasets generated at FZJ through HANAMI.<br><br>More details about the outcomes and results are given in D5.5. |
| Supercomputer's access | Access granted for the Japanese researchers to JURECA-DC through the VSR compute project "Improved Diagnostics of Respiratory Flows Using a Lattice-Boltzmann Method and Machine Learning Techniques" – duration: 05.2024 until 04.2025<br>• JURECA DC Module CPU: 1.76 million core-h<br>• JURECA DC Module GPU: 2.60 million core-h<br><br>Compute time extension (05.2025-04.2026) submitted on 17.02.2025, awaiting response.<br>• JURECA DC Module CPU: 1.22 million core-h<br>• JURECA DC Module GPU: 1.57 million core-h<br><br>Development access will be requested for JUPITER (JEDI access already available)<br><br>Access to FUGAKU: 1.50 million core-h |
| Leverage actions | The team has designed 1 proposition and applied to the Promotion of Joint International Research (International Leading Research) category of the Grants-in-Aid for Scientific Research (KAKENHI)<br>• PI: Makoto Tsubokura, RIKEN/R-CCS<br>• Andreas Lintermann acts as an International Joint Researcher |
| Future plans | Prof. Makoto Tsubokura will visit the FZJ to discuss further collaboration on 03.03.2025<br>Negotiations are ongoing to have a visiting researcher contract at R-CCS<br><br>HANAMI travelling grant requested on 07.2024 by M. Rüttgers for 2 weeks<br>• Visit from researcher planned in 04.2025 - feasibility and other details to be discussed with Hanami organizing team. |

| | |
|---|---|
| | • Visited laboratory: Complex Phenomena Unified Simulation Research Team, Kobe, Japan<br><br>Codes<br>• Discussing the portability of the *m-AIA* code on the Fugaku supercomputer<br>• Running the developed tools on the Fugaku supercomputer<br>• Effective work will start in 04.2025<br><br>In the new compute time proposal (05.2025-04.2026), a sub-project targeted at infection risk analysis for trans nasal-cavity flow is introduced:<br>• Combination of internal and external flow domain to numerically simulate the process of inhalation of viral particles (droplets containing viral matter)<br>• Simulations will be performed with *m-AIA* solver. Alex Krochak will receive training from *m-AIA* developers at RWTH Aachen and work on this subproject if approved.<br>• Successful project would provide data-driven assessment on probability of inhalation of viral particles by healthy patients in environments such as waiting room or public transportation. |

# 3. WP6 HPC for future materials design

High-performance computing (HPC) is used to study and optimize diverse materials properties to support the development of sustainable energy technologies. Simulations enable new dimensions in materials design through increased system complexity, higher accuracy, and improved computational approximations.
By combining HPC with high-throughput workflows and materials informatics, this effort aims to address major societal and technological challenges.
HANAMI strengthens EU–Japan collaboration and improves materials sustainability for energy production and storage. It also strengthens the EU/Japan joint development of extremely scalable numerical libraries and innovative software that may enable future frontier applications.

HANAMI pushes the frontiers of in silico simulations of advanced materials, ensuring interoperability, efficient use of the most powerful computing systems, and the sharing and advancement of optimized codes developed in Europe and Japan. Together, these actions support execution at scale, enhance future frontier applications, and help identify emerging challenges and opportunities for materials research in an evolving HPC ecosystem.

## Project 1: Sustainable materials for photovoltaics and energy storage

| | |
|---|---|
| Objectives | **T6.1 - Sustainable materials for photovoltaics**<br>CNR, RIKEN, Yokohama City University, The University of Tokyo<br>○ Characterize more sustainable materials for perovskite-based solar cells (PSCs), in particular Pb-less and Pb-free PSCs.<br>○ Calculate the interface and GBs from first-principles combining such calculations with large-scale quantum chemistry ones to study their impact on the devices and to the assembling of the active interfaces in tandem cells to predict how the stress may alter the optoelectronic features of the final PSC.<br>○ Optimize the codes in the Japan and EuroHPC machines for efficient calculation in large relevant in perovskite-based solar cells with a particular effort in Distributed solver in large matrix Bethe-Salpeter equation.<br><br>.<br>**T6.2 - Electrochemistry and battery research from first principles**<br>ICN2, CNR, FZJ, NIMS, University of Tsukuba<br>○ The groups in Japan have employed DFT methods to electrochemical problems. Japan is advanced in the formulation of theoretical methods to study the electrified electrode-electrolyte interface (Effective Screening Medium (ESM) by Otani, and Sugino)<br>○ The EU team is expert in the development of DFT methods and their implementation on efficient codes (SIESTA). They have also developed methods to study the electrified interface based on alternative approaches (Non-Equilibrium Green's Functions). |

| | |
|---|---|
| | ○ HANAMI implements the ESM method in SIESTA, to improve the realism of the simulations by introducing a continuum approach for the electrolyte<br>○ HANAMI optimizes the code in the Japan and EuroHPC machines and demonstrate efficient and relevant calculations of the electrified interface in battery materials.<br><br>**T6.3 - Hydrogen storage: adsorption, desorption, reaction barriers from QMC**<br>CNRS, NIMS<br>○ Evaluate the chemical binding energy of hydrogen-bonded systems by employ the TurboRVB code, which implements efficient quantum Monte Carlo (QMC) algorithms and which also includes a built-in path integral molecular dynamics driver. Main developers: Michele Casula (CNRS), Kosuke Nakano (NIMS)<br>○ Obtain highly accurate reaction barriers from QMC simulations including nuclear quantum effects from predictive calculations from first principles<br>○ Combine QMC with Machine Learning to develop fast and accurate potential energy surfaces, and enhance the portability of TurboRVB towards HPC machines thanks to an efficient CPU/GPU parallelization (the workflow manager is TurboGenius) |
| Working process and collaboration format | Meetings online and in person meetings (HLS1 Barcelona) discussing first steps for Pb-free photovoltaic project with Yokohama University Partner (K. Yamashita)<br><br>Online and in person meeting CNR- Riken Partner (W. Dawson) discussing reduced precision benchmark for Yambo and TurboRVB codes. Actions planned.<br>• In person meeting (HLS1 Barcelona, Jan 14th 2025) discussing details of the implementation of ESM in SIESTA, with Tsukuba University Partner (M. Otani)<br>• Periodic online meetings between the ICN2 team and Tsukuba University Partner (M. Otani) on the implementation of ESM in SIESTA.<br>• TurboRVB: weekly online meetings with Kosuke Nakano (NIMS)<br><br>Kosuke Nakano visits the researchers in France (Sorbonne U, CNRS) in September 1-8 2024 and in January 27-30 2025<br><br>Joint publications with CNR-Japanese partners:<br>• Unveiling the Origin of High Air Stability in PbS QD/ZnO Nanowire Heterojunction Solar Cells, submitted, ACS Applied Energy Materials, **Giacomo Giorgi**, Takaya Kubo, et al.<br>• Hydrogen liquid-liquid transition from first principles and machine learning, submitted to PRB, arXiv preprint arXiv:2502.02447, G. Tenti, Bastian Jäckl, **Kosuke Nakano**, Matthias Rupp, **Michele Casula**<br>• Planned Book Project: “Computational Modelling for Advanced Photovoltaics: Materials, Interfaces, and Phenomena for Beyond-Silicon Solar Cells” (Elsevier) as part of the “Theoretical and Computational Chemistry” book series. Edited by **Giacomo Giorgi** (University of Perugia), Sergei Manzhos (Institute of Science Tokyo), and others. |

| | |
|---|---|
| | Planning a material science workshop to be held in Paris in November 2025. Additional funding granted from CECAM-FR node.<br><br>**Recruitment :**<br>• Task 6,1: Hired 2 Years Postdoc Position at CNR Dr. Costanza Borghesi. Theme: Photovoltaic application and enabling Yambo code to solve large excitonic matrixes<br>• Task 6.2: Hired 2 Years Postdoc (Dr. Nils Wittemeier) at ICN2. Start date: Oct 1, 2024. Theme: "Implementation of the EMS method in SIESTA"<br>• Task 6.3: 2 Postdoc Positions at CNRS started in May 2024 and ending in July 2025. Theme postdoc 1: development of QMC data generation techniques adapted to the training of atomistic potentials by machine learning. Theme postdoc 2: development of innovative techniques to compute lattice vibrations in hydrogen-rich compounds, based on machine learning interatomic potential built on top of QMC data. |
| Supercomputer's access | **Access in Supercomputers in Japan:**<br><br>➢ **Yambo Trial Access** Project, project Yambo Scale: hp240326 through HPCI access<br>Duration: 09.2024 for 6 months. Maximum of computing hours: 100000 node-hours<br>• Deployment and benchmarking of the Yambo code have been conducted.<br>• A scaling benchmark using GCC compilation demonstrated good scalability.<br>• Additional benchmarks with Fujitsu compilation are ongoing.<br>• A report, including the compilation recipe and scaling benchmarks, is in preparation.<br>➢ **Fugaku Project Period-A of FY2025** – "Exascale and sustainable materials simulations through extremely scalable libraries and innovative software" was submitted and recently accepted; project number hp250100 through HPCI access<br>Duration: 1 year starting April 1st 2025. Computing hours awarded: 6 Million node-hours (PI E. Di Napoli)<br>➢ **TurboRVB Regular Access Project**, project number hp240033 through HPCI access<br>Duration: FY2024 (01.04.2024 - 31.03.2025) Maximum of computing hours: 5M nh<br>Goal: Development of accurate QMC strategies to generate accurate training sets for machine learning<br>➢ **TurboRVB Regular Access Project,** project number hp250031 through HPCI access<br>Duration: FY2025 (01.04.2025 - 31.03.2026)<br>Goal: First-principles diffusion Monte Carlo calculations with TurboRVB beyond the Coupled Cluster accuracy.<br><br>**Access in Supercomputers in Europe** |

| | |
|---|---|
| | ➢ **TurboRVB Regular Access Project,** project number A0170906493 through GENCI access<br>Duration: 01.11.2024 - 31.10.2025. Maximum of computing hours: Rome TGCC (6.5M core hours), SkyLake TGCC (1M core hours), Jean-Zay IDRIS GPU V100 partition (0.72M GPU hours), Jean-Zay IDRIS CPU partition (0.48M CPU hours)<br>➢ **Yambo: ISCRA-B project Proposal** ID: IsB30_EISD 1.6M core hours on LEONARDO BOOSTER (CINECA, Italy). From 01/01/2025 to 01/01/2026<br>➢ **Siesta: Access to 16 out of 17 available EuroHPC JU partitions** (benchmark access to 15 partitions, development access to Deucalion ARM, regular access to VEGA CPU). Participation in JUREAP. Access granted to MareNostrum5 (BSC, Spain) for 4M core hours from 1/3/25 to 30/6/25 |
| Leverage actions | The team has designed 2 propositions and submitted them.<br>➢ Extreme scale access EuroHPC proposal submitted on 04.2024 and **granted on 10.2024 till 10.2025.** PI: Michele Casula (CNRS), HANAMI project at the core of the proposal<br>➢ ISCRAB proposal – submitted on 01.2025. PI: Giacomo Giorgi (CNR), HANAMI project at the core of the proposal. The proposal under review. |
| Future plans | **HANAMI travelling grant** requested on 06.2024<br>• Visit from researcher (Giorgi, Varsano, Borghesi) planned in 06-07.2025, 2-4 weeks; visited laboratory: Yamashita Lab (Yokohama, JP).<br>• Visit of CNRS team (Casula, Raghav, Cherubini) planned in 04.2025, 2 weeks; visited laboratory: NIMS (Tsukuba, JP).<br>• Two visits of ICN2 postdoctoral researcher to Otani group (Tsukuba, JP) in 03/25 and 01/26, each of them 1 month<br><br>**Workshop** organization around WP6 topics involving both European and Japanese community. (Fall 2025). Extra funding from CECAM granted.<br><br>**Action on codes :**<br>• Yambo<br>  • Porting and benchmark campaign on Fugaku supercomputer (completed with GCC compilation in Jan. 2025, ongoing with Fujitsu compilation)<br>  • Exploration of performance of different solvers in both European and Japanese machines (slepc, magma, ChASE)<br>  • Exploration of precision reduction in collaboration with RIKEN (started in Feb. 2026)<br>• TurboRVB<br>  • Portability of workflow manager TurboGenius across different (European and Japanese) HPC platforms<br>  • Exploration of different machine learning schemes for QMC-derived interatomic potentials<br>• SIESTA<br>  • Porting of ESM to the most recent version of SIESTA (version 5).<br>  • Porting, benchmarking and deployment of SIESTA 5 in EuroHPC systems with the same architecture as FUGAKU (eg. Deucalion CPU ARM).<br>  • Porting, benchmarking and deployment of SIESTA 5 in FUGAKU. |

## Project 2: Exascale Materials Science simulations through extremely scalable libraries and innovative software

| | |
|---|---|
| Objectives | **T6.4 - Numerical linear algebra framework for Materials Science**<br>FZJ, RIKEN, CEA, CNR, University of Tokyo<br>○ Standard framework for large-scale numerical linear algebra libraries development<br>○ Provides a common platform for developers and users to access and utilize various numerical libraries and data structures<br>○ Promotes interoperability and collaboration among the different supercomputing centres and research groups making up the EU-Japan landscape;<br>○ Enables researchers to easily benchmark and evaluate the performance of different parallel algorithms<br><br>**T6.5 - Non-equilibrium charge-carrier dynamics in 2d-materials**<br>FZJ, RIKEN, CEA, CNR<br>○ Development of parallel NEGF & interfacing BigDFT (Massively parallel solver with electron-phonon and electron-photon interactions)<br>○ Implement a framework for the representation of block sparse (with dense blocks) data operating close to peak memory bandwidth and tailored to accelerated platforms.<br>○ Integrate both data framework and abstraction interface in MS code such as BigDFT and libNEGF<br><br>**T6.6 - Enhancing Materials Science scalability through innovative block sparse libraries**<br>FZJ, RIKEN, CEA, CNR<br>○ Extend the scaling of BigDFT by progressively combining the current features of the code with ongoing developments in tasks 6.4<br>○ Combine multiple numerical methods featuring a hierarchy of implementation that can be automatically adapted to current and feature supercomputing platforms.<br>○ Enhance the capabilities of the simulation software and will extend the scope of linear-scaling electronic structure methods and quantum transport to other computer codes and formalisms<br>○ Extend the block matrix representation of NTpoly in the dense format of DBCSR and include the Fermi Operator Expansion (FOE) approach in the new library which would employ block sparse DBCSR representation to benefit from GPU acceleration<br>○ Apply the Kernel Polynomial Methods on-top of the FOE approach to further reduce the number of Chebyshev polynomials to be calculated. |
| Working process and | Regular meetings with Japanese researchers<br>• Monthly exchanges with FZJ and RIKEN on ChASE, EigenExa and the ELSI platform |

| | |
|---|---|
| collaboration format | • Access to Gitlab based repositories for the exchange of information through the creation of Gitlab issues and merging requests<br>• Exchange of additional messages and information through a Slack workspace.<br>• Weekly meeting with CEA and RIKEN in the framework of BigDFT/CheSS/NTpoly developments<br>• New PhD student in collaboration with Tokyo University on efficient usage of BigDFT basis sets<br><br>**Other onsite meetings and workshops with Japanese researchers**<br>• Workshop in Forschungszentrum Juelich, Germany – March 13-15, 2024. Participants : FZJ and RIKEN-CCS<br>• Working visit in Kobe (11.2023) by L. Genovese and of W. Dawson in Grenoble (05.2024) on the topic 'HPC Workflows in Large scale Calculations'<br>• Visit of W. Dawson in Grenoble for 3 weeks in November 2024<br>• Visit of Dr. A. Pecchia to Riken 20th April - 2nd May 2025<br>• Visit of Dr. Imamura to Forschungszentrum Juelich from 11.02 to 13.02.2025<br>• Planning of a WP6 workshop to be held in Paris. Additional funding granted from CECAM-FR node.<br><br>**HANAMI recruitment:**<br>Task 6.4: Hired 2 Years Postdoc Position at Forschungszentrum Juelich—Juelich Supercomputing Centre. Dr. Clement Richefort. Theme: Integrate ChASE with the Yambo code and further develop ChASE to solve pseudo-Hermitian eigenproblems. Develop a parallel framework for the seamless integration of Material Science codes with Numerical linear algebra libraries.<br><br>Task 6.5: Position awarded for a 2 Years Post Doc Position at CNR-ISMN (Interview completed on 14/02/2025). Theme: Perform transport simulations of 2D $MoS_2/WS_2$ bilayers for electronics and photovoltaic properties, probing especially the role of S-vacancies. |
| Supercomputer's access | **Supercomputers access in Japan**<br>• Access granted for FZJ team (for use with ChASE and EigenExa) to Fugaku through HPCI access – duration: 10.2023 until 09.2024. Maximum of computing hours: 3,200,000 node-h<br>• Access granted to FZJ team (for use with ChASE and libNEGF) to Wisteria through JHPCN – duration 05.2024 until 04.2025<br>• Access granted to CEA team (for use with BigDFT and Genesis) to Wisteria through JHPCN – duration 05.2024 until 04.2025<br>• Wisteria workflow calculations designed and running.<br>• Access granted to FUGAKU thanks to successful proposal on HPCI PA-FY2025. Duration: from the 1st April 2025 - 31st March 2026 - Granted computing hours: 5,960,088 nh.<br><br>**Supercomputers access in Europe**<br>• Access to be granted for WP6 P2 Japanese researchers to JUWELS and JUPITER through bilateral MoU FZJ and RIKEN/R-CCS<br>• Access granted to Leonardo for benchmark purposes for BigDFT and CheSS |

| | |
|---|---|
| | • Access granted on LUMI for development project around the BigDFT GPU acceleration. |
| Leverage actions | The team has designed 1 proposition to extend its funds:<br>• Visit of Dr. William Dawson (RIKEN) in France in November 2025: 3 weeks visit at the CEA, funded by the program of the French Embassy |
| Future plans | **Workshop** organization around WP6 topics involving both European and Japanese community. (Summer 2025)<br><br>**HANAMI travelling grant** requested on 06.2024, 8 weeks<br>• Visit from researchers from FZJ planned in 03.2025 and 03.2026<br>• Visit to RIKEN-CCS, Kobe, Japan by CEA planned in 2025.<br>• Visit from researcher (Dr. Pecchia) planned in April 20$^{th}$ April - 2$^{nd}$ May 2025, Riken Lab (Kobe, JP).<br><br>**Codes**<br>• Discussing the code integration and portability on Fugaku supercomputer and planning for the FUGAKU-NEXT project<br>• Effective work starting on 12.2024 with the hiring of a postdocs on a HANAMI funded position to work on task 6.4.<br>• BigDFT interoperability with NTpoly and Genesis in the context of complex HTC workflows on large supercomputers<br>• Design of a prototype workflow in the context of interaction between BigDFT and libNEGF. |

# 4. Conclusion

HANAMI has achieved concrete collaboration with Japan through regular meeting and discussions to follow-up the scientific work to be achieve and design the future plans. All the researchers have also access to supercomputers facilities on both regions, thanks to the established collaborations. These tables will be updated every 6 months (except the objectives part where it refers to the DoA established objectives).