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

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DELIVERABLE 1.9

Follow-up of the scientific collaborations with Japanese partners - 4

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Version History

Revision	Date	Editors	Comments
1.0	11.02.26	France Boillod-Cerneux (CEA)	Template to retrieve the HANAMI work packages information.
1.1	16.02.26	Daniele Varsano (CNR)	Updated info for WP6 in general and Task 6.1.
1.2	03.03.26	Edoardo Di Napoli (FZJ)	Updated info for project 2 WP6 and task 6.4 in particular
1.3	10.03.26	Berk Hess, Umair Sadiq, Erik Lindahl (KTH)	Updated info for project 1 in WP5
1.4	20.03.26	Michele Casula (CNRS), Fabio Affinito (CINECA), Edouard Audit (CEA)	Review and correction
2.0	24.03.26	France Boillod-Cerneux, Christophe Calvin (CEA)	Finalizing the document (proof reading and f.ormat)

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 deliverable is a very short summary of scientific work package, asked by EuroHPC. The format is required (by EuroHPC) to be very short, and in a form of Table/bullet points.

This deliverable is very close to D1.8, as D1.9 gives the overview of work done in February 2026 while D1.8 gives an overview of the work done in August 2025. During this period, the researchers kept collaborating with Japan but were also strongly focused on the multiple events organized by HANAMI (workshops, high level symposium, sustainability events, ...). This document will serve as a basis to highlight HANAMI collaboration with Japan, and will be updated in August 2026, leading to D1.10.

For more details about each scientific project, we invite the reader to consult the deliverables written by WP4, WP5 and WP6 respectively as well as the technical report delivered for the month 18 review.

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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** Partners: BSC, DKRZ, RCCS, NIES 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, including Miyabi, Fugaku and Marenostrum 5, and developed a strong collaboration connecting Japanese and European efforts on weather and climate model development. HANAMI has streamlined a collaborative effort for the future in porting European and Japanese models such as EC-Earth4 and Nicam/COCO to the HANAMI workflow and assessing their replicability, scientific skill, and computational performance on European and Japanese supercomputers. Additionally, we have established an active collaborative engagement in a shared GitLab and vivid exchange via slack and email, where developments of the HANAMI workflow, the pyhanami diagnostics suite, and the replicability test are discussed and continuously developed together. Visits and exchanges:

	• After her long stay at JAMSTEC in May 2025, Marta Alerany continued collaborating with the host group via email exchanges, particularly with Masuo Nakano, building on their expertise to further develop the work on projection skill evaluation initiated during the visit. Marta Alerany's stay resulted into common dissemination activities beyond her time at JAMSTEC, and the development of relevant diagnostics that have been added to the pyhanami suite. Conferences and international workshops: • Kai Keller co-chaired with Chihiro Kodama and others a session at AOGS annual meeting 2025 in Singapore: "Weather and Climate Studies with High Resolution Earth System Models and High Performance Comuting" • Talks of Marta Alerany and Kai Keller at the HANAMI HLS2 • Accepted abstract for presentation at the EGU GA 2026 from Marta Alerany • Presentation of a virtual poster at the CMIP7 community workshop in Kyoto (March 2026) from Marta Alerany (pyhanami) and Kai Keller (Replicability test) • Joint session at the AGU/JpGU meeting in Chiba 2026: "Weather and Climate Studies Using High-Performance Computing: With a Special Session on HANAMI". Conveners: Chihiro Kodama, Hirofumi Tomita, Joachim Biercamp, Samuel Hatfield, Mario Acosta, and others.
Leverage actions	• Computing resources in Japan: The application of the joint proposal to the JHPCN international project has been awarded – project name: ReplicaEUJP. Computing hours at Miyabi-c: 48,664 and Miyabi-G: 10,815 • Publication in a scientific journal - Geoscientific Model Development (Gmd) – DOI:10.5194/gmd-18-10221-2025 – "Replicability in Earth System Models" - Kai Keller, Marta Alerany, Mario Acosta
Supercomputers acces	• Access to Fugaku thanks to the EuroHPC-R-CCS Letter of Intent • Access and computing hours on Fugaku provided from our Japanese partners: • "Artificial Intelligence for Life and Science Simulations on Full-scale of Fugaku" PI: Mohamed Wahib (total: 3,400,000 Node hours in project for shared usage) – October 2025 until March 2026 • Development access on Marenostrum5 - duration: 09.2025 until 12.2025 - Maximum computing hours (node hours): 4000 • Access granted for the Japanese researchers to LUMI through bilateral MoU CSC and RIKEN/R-CCS – duration: 05.2024 until 04.2026 - Maximum of computing hours: 40000 • Access granted for the Japanese supercomputer Miyabi - duration until 2026-03-31 – CPU: 48,664 node hours / GPU: 10,815 node hours.
Future plans	• We plan two more joint publications in scientific journals about the pyhanami diagnostics suite and the HANAMI generic workflow. Those will be joint publications with authors from European and Japanese HANAMI partners. • We are currently conducting 100-member climate simulation ensembles with NICOCO (20 years, pre-industrial control – pi-control) on Fugaku, Miyabi-C, and Marenostrum5. We target to apply the HANAMI developed replicability

	methodology to test for statistical differences in the climates of the models on the different supercomputers.

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

Objectives	**Task 4.2: High-Performance Climate and Weather benchmark** DKRZ, BSC, ECMWF, CSC, NICAM ○ Extend the existing test cases in HPCW; assistance with implementation of NICAM-DC (Japanese atmospheric dynamical core) into HPCW; general maintenance and preparations for first open-source release of HPCW. ○ Preparing HPCW for MN5 deployment. ○ Extend NICAM-DC benchmark in HPCW to higher resolution test cases, investigate other Japanese models such as SCALE for inclusion in HPCW to complement NICAM-DC. ○ 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 by online exchange on Japanese HPCW components (such as the NICAM code). Visits and exchanges occurring in this period • HANAMI HLS2: Hisashi Yashiro (NIES) and Hirofumi Tomita (R-CCS) attended in person, Chihiro Kodama (JAMSTEC) attended online
Supercomputers access	The researchers have now access to Fugaku thanks to the EuroHPC-R-CCS Letter of Intent.
Future plans	• Deep dive on performance of HPCW components on Fugaku, taking advantage of new LoI computing project. Visits and exchanges planned in 2026: • Joint session accepted to JpGU, May 2026 with Hirofumi Tomita (R-CCS), Hisashi Yashiro (NIES), and Chihiro Kodama (JAMSTEC). Kai Keller (BSC) and Sam Hatfield (ECMWF) confirmed attending. • Sam Hatfield (ECMWF) will visit JAMSTEC in Yokohama early June 2026 to hold collaboration discussions and give a seminar, hosted by Chihiro Kodama.

Objectives	**Task 4.3: The University of Warsaw Lagrangian Cloud Model (UWLCM)** Partners: University of Warsaw, University of Hyogo, RIKEN ○ Develop Lagrangian ice microphysics in UWLCM based on the SCALE-SDM implementation ○ Optimize modelling of condensation and deposition in Lagrangian microphysics of UWLCM by developing an adaptive sub stepping algorithm. ○ Deploy UWLCM and test its scalability on different supercomputers.

	○ Optimize UWLCM memory usage
Working process and collaboration format	Agnieszka Makulska and Piotr Dziekan visited University of Hyogo and RIKEN in September 2025. The two-week visit helped specify plans for optimizing and extending Lagrangian microphysics methods. The collaboration continues, in remote with regular online meetings. On site and online meeting with Japanese partners during HLS2 in December 2025. Agnieszka Makulska applied for a RIKEN scholarship for a two-month visit.
Supercomputers acces	The team has now access to Fugaku thanks to the EuroHPC-R-CCS Letter of Intent. Access to Helios and Athena (Cyfronet center in Cracow, Poland) for UWLCM development.
Future plans	○ Test the developed adaptive condensation/deposition substepping algorithm in simplified (parcel) and realistic (LES) simulations. Prepare a manuscript about this research. ○ Continue implementation of ice microphysics developed at the Univ. Of Hyogo: add anisotropic ice crystals. ○ Run UWLCM on multiple nodes of Fugaku (single-node runs already performed).

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** KTH, R-CCS, The Tokyo institute of technology ○ 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 ○ 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. **T5.2 - Data-driven biomolecular modelling & simulation** KTH, R-CCS, RIKEN BDR, University of Groningen, Nagoya University ○ 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 ○ Address the challenges with sensitivity to training domains, investigate possibilities to use "delta-learning", Apply neural networks as a correction ○ 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 • Biweekly meetings with Japanese researchers to collaborate on development efforts • Two shared repositories are maintained (one for stand-alone ExaFMM work, and the other for GROMACS and ExaFMM integration), and both are kept in sync • A general interface between the FMM library and GROMACS has been developed. It has been included in official GROMACS-2026 release. Its already being used by developers of well-known FMM libraries including ExaFMM • GROMACS-FMM experiments have already been performed on the Dardel and ALPS HPC systems, with scaling that is nearly linear up to a couple of thousand ranks • Scaling experiments have been performed with systems containing up-to 45 millions particles • FMM is getting closer to PME (a well-tuned algorithm refined over decades) in terms of performance, and significant progress has been seen most recently; the cross-over point will be identified soon • One conference publication (SC25) has already been made Research visits: • Dr. Muhammad Sadiq visited in Tokyo Tech mid 2025 for joint ExaFMM work • Erik Lindahl gave a talk in the EU-Japan collaboration session at SCAsia on Jan 27 2026, and led the life science lectures of the joint ASEAN HPC school in Kobe Jan 29-Feb 3. New AI4SCIENCE frameworks both in Sweden & Japan to focus on data-driven work and foundation models. We will pursue new collaborations with Profs. Yuji Sugita & Satoshi Matsuoka, and KTH has initiated a new MoU with RIKEN on AI4Science.
Future plans	

	• Joint Publications with Japanese researchers are planned for scalable FMM integrated within GROMACS Planned research visits: • Dr. Muhammad Sadiq to visit Tokyo Tech mid-to-late 2026 for joint ExaFMM work • Prof. Berk Hess visit to RIKEN & Tokyo Tech planned mid-to-late 2026 to finalize work • Prof. Erik Lindahl will visit RIKEN to initiate new AI4Science collaborations and establish a framework to share our extensive experience in GPU acceleration and scaling to aid RIKEN in preparing for Fugaku-next with Nvidia GPUs. 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. This project 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** Barcelona Supercomputing Center (BSC), CSC - IT Center for Science (CSC) • Simulation of cancer genomes and execution of established computational pipelines to identify somatic mutations. • Containerisation of the tools involved in the workflow, following best-practice guidelines and including quality-control steps to assess the limitations of mutation discovery. • Benchmarking of the developed computational pipeline on different supercomputing infrastructures, evaluating memory usage and execution time. • Assessment of the scalability of the workflow to simulate and analyse large populations of cancer patients' interventions to mitigate tumour growth

	T5.4 – Tumour Evolution Simulation Pipelines Barcelona Supercomputing Center (BSC), CSC - IT Center for Science (CSC) • Use of simulated cancer genomes within multiscale cellular simulations to support the development of digital twins of the human body. • Containerisation of the tools involved in the simulation workflow and documentation of the complete pipeline. • Development of personalised intracellular models based on the specific set of somatic mutations identified in each simulated cancer genome. • Evaluation of potential drug interventions within the simulated models to explore possible therapeutic strategies.
Working process and collaboration format	We are actively collaborating with Ai Shinobu and Elisa Dominguez (PRIMe Institute, Osaka University) to develop a shared workflow to study how somatic mutations in cancer lead to changes in cellular behaviour. The collaboration includes: • **Regular meetings** to define a clear step-by-step computational pipeline, from identifying mutations in cancer patients to estimating their potential biological effects. • Development of a **personalised medicine perspective**, where the combined set of mutations of a given patient is analysed within the same simulations and compared against an unmutated reference profile to help evaluate possible therapeutic strategies. • Integration of **classical somatic mutation analysis tools with advanced molecular dynamics techniques**, an area where Dr. Ai Shinobu and Dr. Elisa Dominguez bring strong expertise. • Exploration of **structure-based protein modelling approaches**, including AI-based scoring methods to evaluate mutation effects. • Molecular dynamics analyses provided by our collaborators to study both **structural effects of mutations on proteins** and **disruptions in protein–protein interactions**, which may impact intracellular processes studied by our group. • Joint identification of **practical modelling strategies for the first implementation**, prioritising approaches that are feasible in terms of available data and computational resources.

	As part of this collaboration, we hosted Dr. Ai Shinobu and Dr. Elisa Dominguez at our institution from **15–18 December 2025**, shortly after the HLS2 event in Chamonix, where Dr. Ai Shinobu delivered two invited talks. In parallel, through our collaboration with Mariko Okada (Osaka University), we are preparing a **scientific workshop in Japan** focused on AI, high-performance computing, and biological sciences, with a strong emphasis on interdisciplinary research and biological system modelling, particularly relevant for HANAMI WP5. • The event is expected to host **150–200 participants** and will be organised by Osaka University, RIKEN, Japan Science and Technology Agency (JST), and the HANAMI consortium. • Expected participants include researchers from JST and RIKEN, pharmaceutical companies in Japan, representatives from the Fugaku project, government representatives, and members of the wider scientific community. • The main symposium is tentatively planned for 3 November 2026 in Tokyo, followed by a technical workshop on 5 November 2026 in Kyoto. • Four speakers for the main symposium have already been identified by the Japanese collaborators, covering topics such as genomics, AI-driven drug discovery, and single-cell analysis, while keynote and European speakers are still being confirmed. Finally, in collaboration with Eliott Jacopin (RIKEN), we are contributing to the organisation of activities related to an event within the Trillion Parameter Consortium (TPC), where teams work with HPC experts to optimise and accelerate scientific and AI applications on advanced computing systems such as GPUs.
Future plans	• Internship of José Carbonell at Osaka University, hosted by Ai Shinobu, planned for April–May 2026. • Completion of the shared computational pipeline integrating molecular dynamics techniques with intracellular modelling, enabling a co-designed Europe–Japan workflow and exploring opportunities for joint scientific publications.

	• Organisation and delivery of the scientific workshop in Japan, in collaboration with Mariko Okada, planned for later in 2026.

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** FZJ, RIKEN Kobe University ○ 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 ○ 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 ○ Employing deep learning techniques for flow field decomposition to investigate different modes of flow fields **T5.6 - AI-assisted surgery planning and risk assessment of exhaled infectious aerosols** FZJ, RIKEN Kobe University ○ 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 ○ 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 ○ Coupling CUBE simulations of indoor scenarios to a genetic algorithm to optimize the interior design of clinical facilities
Working process and	Monthly meetings with Japanese researchers to exchange progress of the Joint Laboratory for Extreme Scale Computing (JLESC) Project “Deep Neural Networks for CFD Simulations”

collaboration format	Further online meetings to achieve the following: • Joint publication about physics-informed neural networks for flow predictions • Joint publication about the decomposition of flow fields with machine learning • 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 • Recent publication on experimental-data-driven boundary conditions for LBM simulations - this application can be extended for boundary conditions for respiratory flow simulations • Another paper is currently in review to advance the use of CFD in rhinology Codes development with HANAMI (started in 04.2025) • Discussing the portability of the *m-AIA* code on the Fugaku supercomputer • Running the developed tools on the Fugaku supercomputer • More details about the outcomes and results are given in D5.5.
Supercomputer's access	Compute time extension (05.2025-04.2026) submitted on 17.02.2025 is granted • JURECA DC Module CPU: 1.22 million core-h • JURECA DC Module GPU: 1.57 million core-h Development access will be requested for JUPITER (JEDI access already available) Access to FUGAKU: 1.50 million core-h New extensions to JURECA-DC has been submitted in February 2026: • JURECA DC Module CPU: 1.41 million core-h • JURECA DC Module GPU: 2.25 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) – waiting for the answer • PI: Makoto Tsubokura, RIKEN/R-CCS • Andreas Lintermann acts as an International Joint Researcher
Collaboration activities	HANAMI travelling grant • Oleksandr Krochak from FZJ has visited RIKEN-CCS and Kobe university in June 2025 • m-AIA code has been ported to Fugaku with preliminary tests carried out. Future joint research collaborations were discussed with members of Complex Team. • Negotiation of visiting researcher contract at R-CCS
Future plans	The next JLESC workshop will be organized at JSC in Juelich, Germany (https://jlesc.github.io/) Several members of Complex Team from Riken-CCS are invited and plan on coming. Both FZJ researchers and members of Complex Team under Prof. Tsubokura will be present at ECCOMAS in the summer of 2026 in Munich, Germany. This opportunity is planned to synchronize in person and build/plan future joint research activities.

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** CNR, RIKEN, Yokohama City University, The University of Tokyo ○ Characterize more sustainable materials for perovskite-based solar cells (PSCs), in particular Pb-less and Pb-free PSCs. ○ Submission of a joint paper (CNR-Yokohama University) on Protective Role of Oxides on Pb-free Halide Perovskite Surfaces. ○ 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. ○ 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. ○ Integration of the Chase library in Yambo code (together with T6.4) ○ Second benchmark campaign of Yambo code in Fugaku after refactoring of the algorithm for the response function (gain 2x in time to solution) **T6.2 - Electrochemistry and battery research from first principles** ICN2, CNR, FZJ, NIMS, University of Tsukuba ○ 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) ○ 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 ○ HANAMI optimizes the code in the Japan and EuroHPC machines and demonstrate efficient and relevant calculations of the electrified interface in battery materials. **T6.3 - Hydrogen storage: adsorption, desorption, reaction barriers from QMC** CNRS, NIMS ○ 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) ○ Obtain highly accurate reaction barriers from QMC simulations including nuclear quantum effects from predictive calculations from first principles ○ 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. The **HANAMI Materials Science Workshop**, held in November 2025 in **Paris**, was a key event for strengthening EU–Japan collaboration within the HANAMI initiative. The workshop gathered 25 invited speakers from leading European and Japanese institutions. Japanese invited speakers included: • **Tomomi Shimazaki** (Yokohama City University) • **Takao Kotani** (Tottori University) • **Toshiyuki Imamura** (RIKEN Center for Computational Science) • **Ayako Nakata** (NIMS, MANA) • **Azusa Muraoka** (Japan Women's University) • **Terumasa Tadano** (NIMS) The program covered advanced materials science applications, European and Japanese electronic-structure codes, and numerical libraries relevant to both HPC ecosystems. Strategically, the workshop reinforced interoperability discussions, enabled direct exchanges between code developers and HPC centers, and identified concrete follow-up actions in benchmarking and performance optimization. It significantly consolidated the EU–Japan partnership and strengthened the sustainability and long-term impact of the HANAMI collaboration.

	In December, the HLS2 in Chamonix was the occasion for in person meetings with Japanese partners. The materials science track gathered 16 talks with the participation of researchers from Japanese Institutions: Sergei Manzhos (online), Kazuhiro Yabana (Univeristy of Tsukuba), William Dawson (Riken-RCCS, Kobe) and Toshiyuki Imamura (Riken-RCCS, Kobe)
Supercomputer's access	**Access in Supercomputers in Japan:** ➢ **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 Duration: 1 year starting April 1st 2025. Computing hours awarded: 6 Million node-hours (PI E. Di Napoli) ➢ **TurboRVB Regular Access Project,** project number hp250031 through HPCI access Duration: FY2025 (01.04.2025 - 31.03.2026) Goal: First-principles diffusion Monte Carlo calculations with TurboRVB beyond the Coupled Cluster accuracy. **Access in Supercomputers in Europe** ➢ **TurboRVB Regular Access Project** through GENCI access 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) ➢ **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 ➢ **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 **HANAMI visits done until M18:** • Visit of CNR researchers (Giorgi, Borghesi) planned in 06-07.2025, 2 weeks; visited laboratory: Yamashita Lab (Yokohama, JP) and Japan's Women University (Muraoka Lab.). • Visit of CNR researchers (D. Varsano, F. Paleari): visit to Riken-CCS (Kobe) (February 2026) • Visit of CNR researcher (G. Giorgi) to Yamashita Lab (Yokohama, JP) (Dec-2025 - Jan 2026) • Visit of Yoshitaka Tateyama to CNR lab in Modena (February 2026)
Future plans	• 1 visit of ICN2 postdoctoral researcher to Otani group (Tsukuba, JP) in 01/26 for 1 month

	• 3rd Benchmark campaign of Yambo code on Fugaku machine after optimization of Fugaku compiler in collaboration with Riken-CCS • Benchmark of Yambo code for mixed precision calculations exploiting high precision emulators (Ozaki scheme) in collaboration with Riken-CCS. • The visit of K. Yamashita to the CNR laboratory in **Modena**, initially scheduled for February 2026, has been postponed for health reasons and will be rescheduled at a later date. • March 2026: Visit of M. Casula to NIMS, Tsukuba and to RIKEN, Wako, Tokyo for a collaboration with K. Nakano and R. Arita, on the development of TurboRVB (Fortran based QMC code), jQMC (JAX based QMC code) and the study of hydrogen-based materials for energy (superconductors)

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

Objectives	**T6.4 - Numerical linear algebra framework for Materials Science** FZJ, RIKEN, CEA, CNR, University of Tokyo ○ ChASE library extension for pseudo-Hermitian eigenvalue problem has been completed and released. An ArXiv article is available on the extension [http://arxiv.org/abs/2601.10557]. ○ ChASE library has been fully coupled with the YAMBO code to solve both Hermitian and pseudo-Hermitian eigenvalue problems through a targeted interface. ○ Collaboration on including the Ozaki-II scheme into ChASE started in October 2025. Currently ongoing work in implementing a Ozaki mechanism within the polynomial filter of the ChASE library where multiple repeated GEMMS are performed. **T6.5 - Non-equilibrium charge-carrier dynamics in 2d-materials** FZJ, RIKEN, CEA, CNR ○ Development of parallel NEGF & interfacing BigDFT (Massively parallel solver with electron-phonon and electron-photon interactions) ○ Implement a framework for the representation of block sparse (with dense blocks) data operating close to peak memory bandwidth and tailored to accelerated platforms. ○ Integrate both data framework and abstraction interface in MS code such as BigDFT and libNEGF **T6.6 - Enhancing Materials Science scalability through innovative block sparse libraries** FZJ, RIKEN, CEA, CNR

	○ Extend the scaling of BigDFT by progressively combining the current features of the code with ongoing developments in tasks 6.4 ○ Combine multiple numerical methods featuring a hierarchy of implementation that can be automatically adapted to current and feature supercomputing platforms. ○ 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 ○ 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 ○ 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 collaboration format	Regular meetings with Japanese researchers • Monthly exchanges with FZJ and RIKEN on ChASE, EigenExa and the ELSI platform • Access to Gitlab based repositories for the exchange of information through the creation of Gitlab issues and merging requests • Exchange of additional messages and information through a Slack workspace. • Weekly meeting with CEA and RIKEN in the framework of BigDFT/CheSS/NTpoly developments **Other onsite meetings and workshops with Japanese researchers** • Workshop in Forschungszentrum Juelich, Germany – March 13-15, 2024. Participants : FZJ and RIKEN-CCS – this workshop gathered 20 persons • Visit of Dr. A. Pecchia to Riken 20th April - 2nd May 2025 • Visit of E. Di Napoli and C. Richefort in Kobe from October 3rd until October 27 2025 during which the start of the collaboration on the Ozaki scheme took place. • Participation to the HPCASIA of C. Richefort with a poster on ChASE extension to pseudo-Hermitian problems (January 2026) • Participation to ADAC18 (Osaka and Tokyo) by C. Richefort in February 2026
Supercomputer's access	**Supercomputers access in Japan** • Access granted to FZJ team (for use with ChASE and libNEGF) to Wisteria through JHPCN – duration 05.2024 until 04.2025 • Access granted to CEA team (for use with BigDFT and Genesis) to Wisteria through JHPCN – duration 05.2024 until 04.2025 • Wisteria workflow calculations designed and running. • 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. **Supercomputers access in Europe**

	• Access to be granted for the Japanese researchers to JUWELS and JUPITER through bilateral MoU FZJ and RIKEN/R-CCS. • 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: • 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 in 2026 is under consideration. **HANAMI travelling grant** requested to make visits in 2026 • Visit from researchers from FZJ planned in 10.2025 and 09.2026 **Codes** • Discussing the code integration and portability on Fugaku supercomputer and planning for the FUGAKU-NEXT project • BigDFT interoperability with NTpoly and Genesis in the context of complex HTC workflows on large supercomputers • 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 meetings, researchers stays (short, medium and long stay), code development, joined publications, co-organization of workshops, 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 are updated every 6 months (except the objectives part where it refers to the DoA established objectives).