HANAMI

Deliverable D1.6

Follow-up of the scientific collaborations with Japanese partners

Funded by the European Union

EuroHPC Joint Undertaking

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D1.6 - Follow-up of the scientific collaborations with Japanese partners

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

Work Package	**1**
Task	1.6
Lead Authors	France Boillod-Cerneux (CEA) Laure Caruso (CEA)
Contributors	All members of HANAMI
Peer Reviewers	Mario Acosta (BSC) Pihla Kauranen (CSC)
Version	2.0
Due Date	31.08.24
Submission Date	29/08/24

D1.6 - Follow-up of the scientific collaborations with Japanese partners

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)

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D1.6 - Follow-up of the scientific collaborations with Japanese partners

Version History

Revision	Date	Editors	Comments
1.0	15.07.24	France Boillod-Cerneux (CEA)	Template to retrieve the HANAMI work packages information.
1.1	01.08.24	HANAMI members	Providing inputs for all work packages
2.0	29/08/24	France Boillod-Cerneux (CEA)	Gathering the work packages presentations and consolidating the deliverable.

D1.6 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 D1.7, D1.8, D1.9 and D1.10.

D1.6 Outlines

- **WP2 – Communication, Dissemination and Exploitation**
- **WP7 – The roadmap for sustainable Europe-Japan collaboration**
- **WP3 – Scientific and technology networking and community building**
- **WP4 – Application development for the climate and weather modelling community**
- **WP5 – Biomedical application co-development to address societal challenges**
- **WP6 – HPC for future materials design**

WP2
Communication, Dissemination and Exploitation

WP2 Communication, Dissemination and Exploitation

- Communication, Dissemination and Exploitation are developed based on an integrated marketing communication approach

- All HANAMI partners are invited to be part of the project community and contribute to different communication actions
  - success stories, testimonials, blog posts, webinars and dissemination of different pieces of information
- The gender dimension is strongly considered within HANAMI

WP2 Objectives

- Define a strategy to communicate and disseminate relevant stakeholders about the project
- Communicate news and facts about the project stakeholders and results
- Promote cooperation between the HPC communities within and between regions
- Communicate the benefits and advantages of the project results
- Cooperate with other EU and Japan-funded projects in the HPC field
- Promote sharing of knowledge and project results to influencers and international networks
- Engage and promote networking among the project target groups

WP2 Communication, Dissemination and Exploitation

Work package leader

Rui Oliveira

HANAMI members

INESCTEC

JÜLICH Forschungszentrum

Universität Stuttgart

HLRS

WP2 Communication, Dissemination and Exploitation

Paula Rodrigues
INESC TEC

Rita Moutinho
INESC TEC

Katherine Cordery
Jülich

Maximilian Tandi
Jülich

T2.1 Project Communication

WP2 Communication, Dissemination and Exploitation

Paula Rodrigues
INESC TEC

Rita Moutinho
INESC TEC

Sophia Honisch
USTUTT/HLRS

Katherine Cordery
Jülich

Maximilian Tandi
Jülich

T2.2 Project Dissemination and Exploitation

WP2 Communication, Dissemination and Exploitation

Rita Moutinho
INESC TEC

Sophia Honisch
USTUTT/HLRS

Katherine Cordery
Jülich

Maximilian Tandi
Jülich

T2.3 Collaboration

WP2 Communication, Dissemination and Exploitation

T2.1 - Project Communication		
M1 01.03.2024 until M36 27.02.2027	INESCTEC	• Production of the visual identity of the project • Development of the website • Creation of the social media accounts • Production of different communication materials to disseminate the project mission, goals and results • Implementation of 3 communication campaigns to reach different target groups and use different communication channels in order to increase awareness about the project and promote engagement with different audiences.

M2.1	Project image, website and social media available	M3 – 05.2024
R2.1	Present the project image and the website of the project	M3 – 05.2024
R2.2	Define the communication, dissemination, and exploitation plan for the project	M6 – 08.2024

WP2 Communication, Dissemination and Exploitation

T2.2 - Project Dissemination and Exploitation		
M1 01.03.2024 until M36 27.02.2027	INESCTEC	• Creation of the dissemination channels • Definition of the stakeholders to be involved • Implementation of a dissemination strategy to disseminate the project results • Definition of KPIs for each activity • Promotion of the publication of scientific articles at international conferences • Dissemination through the website, social media, scientific articles, newsletters, and presentations at different types of events

M2.2	Several communication materials available	M18 – 11.2025
R2.3	Define the collaboration strategy with the Japanese consortium and with other relevant stakeholders	M9 – 11.2024
R2.4	Report about the first half of the project concerning the communication and dissemination activities	M18 – 11.2025

WP2 Communication, Dissemination and Exploitation

T2.3 - Collaboration		
M4 01.06.2024 until M36 27.02.2027	Universität Stuttgart H L R S	Promote collaboration and the sharing of knowledge and experiences, as well as best practices in the identified priority domains between the European and Japanese HPC communities, and leverage this knowledge and the results via collaboration with further initiatives. • Organization of (mainly digital) events with partners and stakeholders • Mapping of the partners; (extended) networks and building new relationships with suitable actors • Representation of the project at scientific conferences, and exhibitions the project partners regularly visit via dissemination material • Participation in events organised by the HPC centres • Dissemination of external calls

M2.3	Several collaborative interactions in place, e.g. events organised by the consortium	M18 – 11.2025
R2.5	Report about the second half of the project concerning the communication and dissemination activities	M18 – 11.2025
R2.6	Report about the implementation of the collaboration plans as defined in D2.3	M36 – 02.2027

WP2 Communication, Dissemination and Exploitation

- Kickoff event in April 2024
  - About 40 attendees in remote, among which 20 Japanese
  - 2 keynotes speakers: Kengo Nakajima and Toshiyasu Ichioka

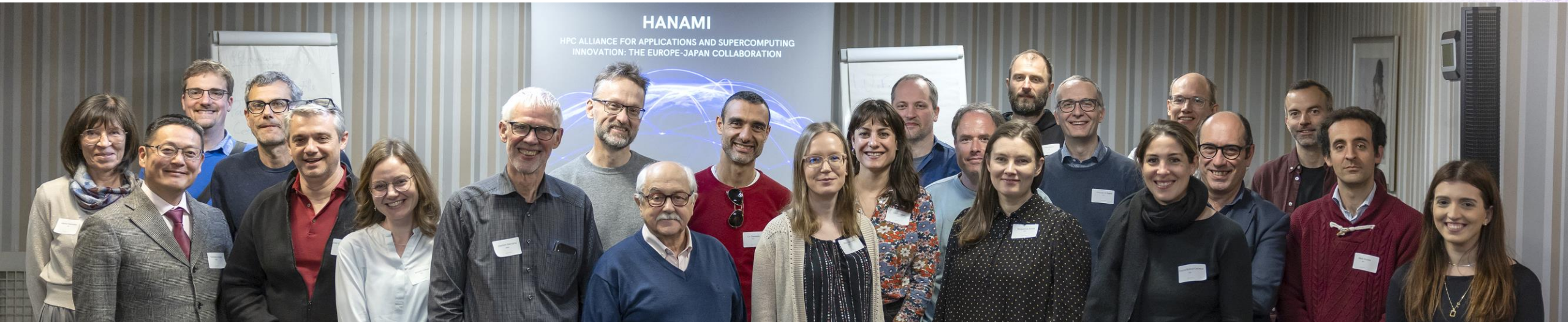
AGENDA HANAMI KICK-OFF MEETING

Location : Hotel Mercure Paris 19 Philarmonie La Villette
Date : Tuesday 23 of April, 2024
Time : 9 to 17.30

Time	Duration	Agenda items	Speaker	Location
8.30 - 9	30'	*Registration*		hall
9 - 9.10	10'	Welcome & Opening	France Boillod-Cerneux *CEA*	plenary room
9.10 – 9.20	10'	Introduction and general presentation of HANAMI project	France Boillod-Cerneux *CEA* Laure Caruso *CEA*	
9.20 – 9.30	10'	RIKEN presentation	Toshiyasu Ichioka *RIKEN*	
9.30 – 9.40	10'	RIKEN and HPCI/U.Tokyo.	Kengo Nakajima *RIKEN/U.Tokyo*	
9.40 – 9.50	10'	WP4 Climate and modeling	Mario Acosta *BSC*	
9.50 – 10.00	10'	WP5 Biomedical	Erik Lindahl *KTH*	
10.00 – 10.10	10'	WP6 Materials science	Edoardo di Napoli *FZJ*	
10.10 – 10.20	10'	WP3 Community building	Edouard Audit *CEA*	
10.20 – 10.30	10'	WP2 Communication	Rita Moutinho *INESC TEC*	
10.30 – 10.45	15'	*Break*		hall
10.45 – 10.55	10'	WP7 Sustainability	Maijastiina Arvola *CSC*	plenary room
10.55 – 11.05	10'	EuroHPC	Catarina Guerreiro *EuroHPC*	
11.05 – 11.20	15'	Question & discussion		
11.20 – 11.55	35'	Future roadmap - *WP7*	Maijastiina Arvola *CSC*	
11.55 - 12.40	45'	Scientific collaborations	WP 4-5-6 + Japanese consortium	parallel session
12.40 - 13.40	1h	*Lunch – group photo*		hall
13.40 - 14.10	30'	Communication & dissemination activities - *needs from all*	Rita Moutinho *INESC TEC*	plenary room
14.10 - 14.50	40'	Communication actions (video shooting, direct meetings...)	WP2	parallel session
14.10 - 14.50	40'	Scientific collaborations	WP 4-5-6	parallel session
14.10 - 14.50	40'	Travelling grants	WP3	parallel session
14.50 - 15.05	15'	*Break*		

WP2 Communication, Dissemination and Exploitation

- Kickoff event in April 2024
  - Video interviews
  - Presentation of each partners of the consortium



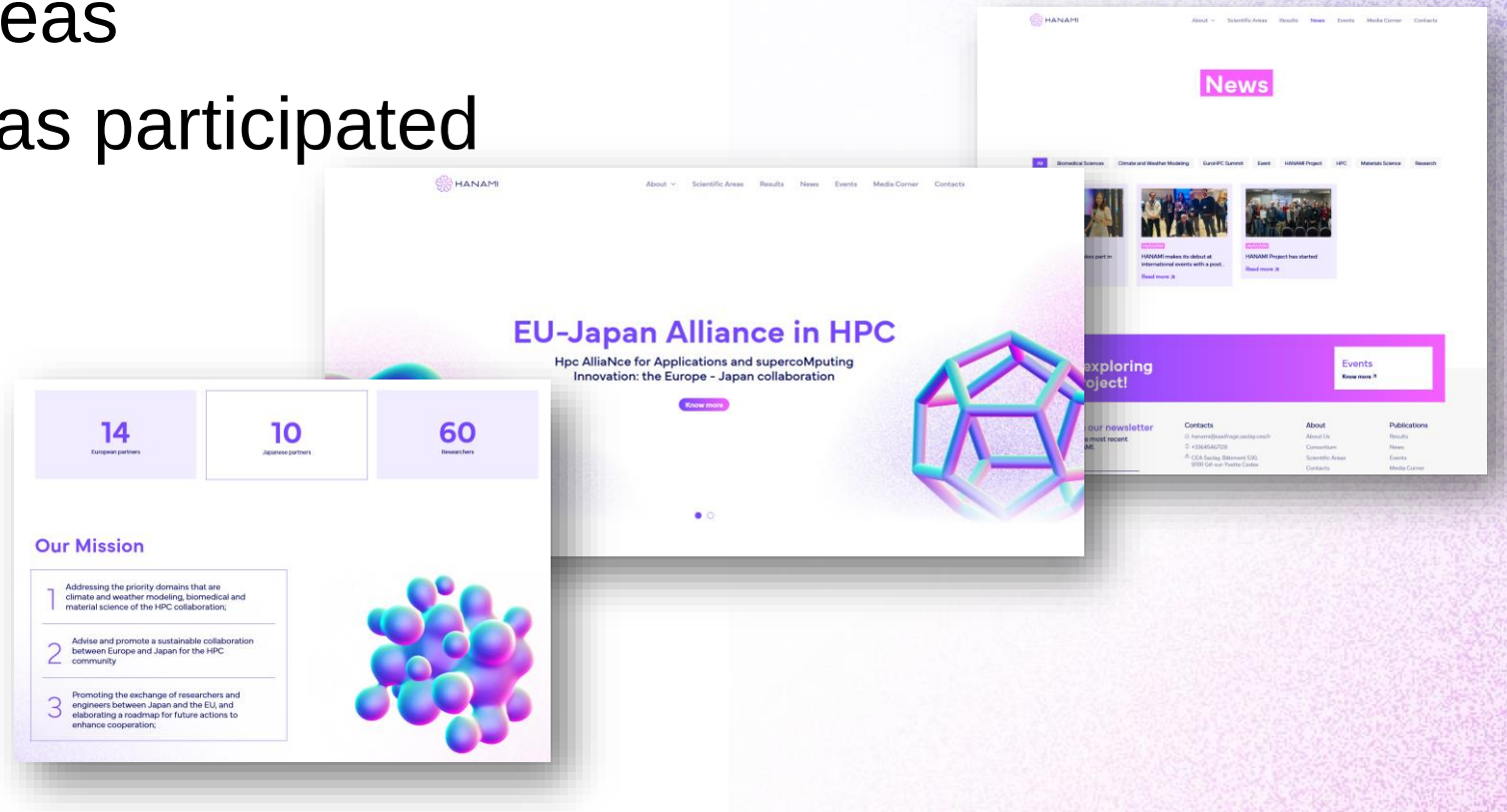
WP2 Communication, Dissemination and Exploitation

First collaboration activities:

- Poster video at EuroHPC Summit 2024, March Antwerp
- Presentation & dissemination of material at ISC 2024, May Hamburg
- Rollup at Teratec Forum 2024, June Paris
- Presentation and dissemintion of material at Workshop on Sustained Simulation Performance, June Stuttgart
- Dissemination of promotional material at International HPC Summer School 2024, July Kobe

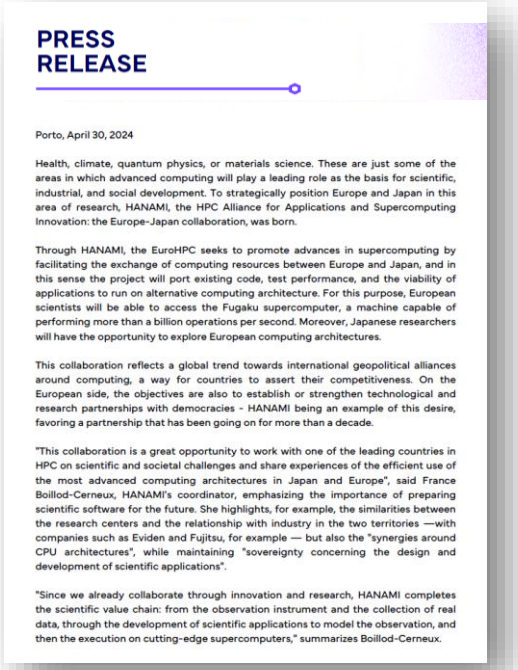
WP2 Communication, Dissemination and Exploitation

- Website is now available at www.hanami-project.com
- Presentation of the overall project
- Presentation of scientific areas
- Events in which HANAMI has participated
- Contact information



WP2 Communication, Dissemination and Exploitation

- Press releases
  - Kickoff meeting
  - Newsletter EU-Japan on June 2024 edition
  - Galileo platform



PRESS RELEASE

Porto, April 30, 2024

Health, climate, quantum physics, or materials science. These are just some of the areas in which advanced computing will play a leading role as the basis for scientific, industrial, and social development. To strategically position Europe and Japan in this area of research, HANAMI, the HPC Alliance for Applications and Supercomputing Innovation: the Europe-Japan collaboration, was born.

Through HANAMI, the EuroHPC seeks to promote advances in supercomputing by facilitating the exchange of computing resources between Europe and Japan, and in this sense the project will port existing code, test performance, and the viability of applications to run on alternative computing architecture. For this purpose, European scientists will be able to access the Fugaku supercomputer, a machine capable of performing more than a billion operations per second. Moreover, Japanese researchers will have the opportunity to explore European computing architectures.

This collaboration reflects a global trend towards international geopolitical alliances around computing, a way for countries to assert their competitiveness. On the European side, the objectives are also to establish or strengthen technological and research partnerships with democracies - HANAMI being an example of this desire, favoring a partnership that has been going on for more than a decade.

"This collaboration is a great opportunity to work with one of the leading countries in HPC on scientific and societal challenges and share experiences of the efficient use of the most advanced computing architectures in Japan and Europe", said France Boillod-Cerneux, HANAMI's coordinator, emphasizing the importance of preparing scientific software for the future. She highlights, for example, the similarities between the research centers and the relationship with industry in the two territories —with companies such as Eviden and Fujitsu, for example — but also the "synergies around CPU architectures", while maintaining "sovereignty concerning the design and development of scientific applications".

"Since we already collaborate through innovation and research, HANAMI completes the scientific value chain: from the observation instrument and the collection of real data, through the development of scientific applications to model the observation, and then the execution on cutting-edge supercomputers," summarizes Boillod-Cerneux.

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HANAMI IS THE NEXT GENERATION OF THE **HPC ALLIANCE BETWEEN EUROPE AND JAPAN**

The HANAMI (HPC AlliaNce for Applications and supercoMputing Innovation) project builds on the EU-Japan Digital Partnership by bringing together research teams representing excellence in High-Performance Computing (HPC) from both Europe and Japan.

HANAMI

This initiative focuses on optimizing HPC applications in domains of common interest for future generations of supercomputing architectures and promoting the use of such supercomputers in the EU and Japan. European and Japanese research centers will collaborate to develop and optimize applications in various scientific fields, with a focus on climate and weather modelling, materials science, and biomedicine. This collaboration builds upon and extends the already established scientific cooperation between the two regions. Joint activities between the European consortium and Japanese research institutes will leverage expertise to develop HPC applications by designing new models, optimizing, developing, and integrating new and ambitious workflows and models to efficiently benefit from pre-exascale and exascale systems deployed or already operational in Europe and Japan. Funded by EuroHPC, the HANAMI project started in March 2024 and will run for 36 months. The project involves about 60 researchers from 14 European organizations and 6 Centers of Excellence for HPC applications (MaX, EoCoE, TREX, RAISE, EsiWACE, and PerMedCoE).
The project, led by the French Alternative Energies and Atomic Energy Commission (CEA), in France, includes 14 European organizations: Barcelona Supercomputing Center (BSC) and Catalan Institute of Nanoscience and Nanotechnology (ICN2), from Spain, CINECA and National Research Council of Italy (CNR), from Italy, Centre national de la recherche scientifique (CNRS), from France, IT Center for Science (CSC), from Finland, Deutsches Klimarechenzentrum (DKRZ), Forschungszentrum Jülich (FZJ), and the High-Performance Computing Center of the University of Stuttgart (HLRS/USTUTT), from Germany, European Centre for Medium-Range Weather Forecasts (ECMWF), from UK, Institute for Systems and Computer Engineering, Technology and Science (INESC TEC), from Portugal, KTH Royal Institute of Technology (KTH), from Sweden, and University of Warsaw (UW), from Poland. The project also brings together 10 Japanese institutions, namely, Japan Agency for Marine-Earth Science and Technology (JAMSTEC), Kyushu University, National Institute for Environmental Studies, National Institute for Materials Science, Research Center for Advanced Science and Technology (RCAST), RIKEN, Tokyo Institute of Technology (TITECH), University of Tokyo, University of Tsukuba, and Yokohama University.

Source: Commissariat à l'Energie Atomique et aux Energies Alternatives https://lnk.bio/HANAMIProject

WP2 Communication, Dissemination and Exploitation

- Future plans
  - HANAMI communication plan M1-M12
    - The goals of the first communication on the campaign are to inform the project audiences about the existence of the project and to communicate news and facts about the initiatives, events and partners of the project with a special focus on the collaboration between both regions.
    -
  - HANAMI participation to SC24
    - Proposal for BoF at SC24 was submitted, focus topic: Building international HPC collaborations across continents to tackle grand challenges: The HANAMI project

WP7
The roadmap for sustainable Europe-Japan collaboration

WP7 The roadmap for sustainable Europe-Japan collaboration

- Establish a wide community of research organizations, research and innovation funders, industrial partners, policymakers, and other collaborative projects and initiatives between EU and Japan to understand the needs and requirements of different stakeholders and ensure community support.
- Define sustainable cooperation structures
- Identify possible national and European funding sources for continued cooperation
- Identify the key exploitable results from the project to be included in the roadmap for sustained cooperation
- Define a roadmap for future cooperation.

WP7 The roadmap for sustainable Europe-Japan collaboration

Work package leader

Maijastiina Arvola

HANAMI members' coordination team

In addition, all HANAMI participants contribute to the sustainability work in their collaborative efforts

WP7 The roadmap for sustainable Europe-Japan collaboration

Pihla Kauranen

Maijastiina Arvola

Sophia Honisch

France Boillod-Cerneux

Laure Caruso

T7.1 **Establishing the EU-Japan community**

WP7 The roadmap for sustainable Europe-Japan collaboration

Pihla Kauranen

Maijastiina Arvola

Sophia Honisch

France Boillod-Cerneux

Laure Caruso

T7.2 **Cooperation structures and sustainable funding**

WP7 The roadmap for sustainable Europe-Japan collaboration

Pihla Kauranen

Maijastiina Arvola

Sophia Honisch

France Boillod-Cerneux

Laure Caruso

T7.3 **Definition of a roadmap for sustained collaboration**

WP7 The roadmap for sustainable Europe-Japan collaboration

T7.1 - Establishing the EU-Japan community		
M1 01.03.2024 until M36 27.02.2027	CSC HLRS Universität Stuttgart cea	• Aim to establish the EU-Japan community, bringing together various stakeholders to understand their needs and ensure support for sustaining collaboration beyond the HANAMI project • Three high-level events will be organized during the project, potentially in conjunction with the scientific symposia (WP3) to demonstrate the value and impact of Europe-Japan HPC collaboration, and discuss the needs and requirements for continued collaboration • The task will also prepare policy papers, maintain relations with policy makers and funders, and address collaboration requirements and priorities. It will interact with several European projects and initiatives, considering supplementary themes like the convergence of HPC and QC.

R7.1	Report about ways to engage policymakers and funders to the cooperation	M4 – 06.2024
M7.1	Three annual high-level sustainability events organized	M36 – 02.2027

WP7 The roadmap for sustainable Europe-Japan collaboration

T7.2 - Cooperation structures and sustainable funding		
M1 01.03.2024 until M28 28.02.2026	cea Universität Stuttgart HLRS CSC	• Investigate different possibilities for sustainable cooperation structures and assess their feasibility (e.g. rules of participation, roles and responsibilities, community engagement methods, gender equality aspects). • Task force to investigate future funding opportunities and different possibilities for sustained funding for the collaboration – proposals in possible funding models for future collaboration

R7.2	Report about possible cooperation structures and funding models ways to engage policymakers and funders to the cooperation	M30 – 08.2026

WP7 The roadmap for sustainable Europe-Japan collaboration

T7.3 - Cooperation structures and sustainable funding		
M13 01.02.2025 until M36 27.02.2027	CSC Universität Stuttgart HLRS cea	• Roadmap defines the overall aim and timeline of the sustained collaboration, targets for sustained collaboration in different thematic areas, Key Exploitable Results that will be sustained beyond the project lifetime (in coordination with WP4-6), key organizations, and proposal on a sustainable cooperation structure and funding model for continued cooperation (based on the analysis in T7.2) • Addresses also thematic areas outside the exact scope of HANAMI, and sets criteria for inclusion of future topics and organizations extending beyond the HANAMI consortium • Addresses the availability of HPC resources for sustained collaboration (linking with the Supercomputing Resource Group in WP1) • The roadmap will be defined based on the outputs from T7.1 and T7.2, outputs of and discussions with other work packages, as well as discussions with strategic stakeholders and HANAMI project management bodies.

M7.2	Agreement on roadmap for sustained cooperation	M36 – 02.2027
R7.3	Report on roadmap for sustained cooperation	M36 – 02.2027

WP7 The roadmap for sustainable Europe-Japan collaboration

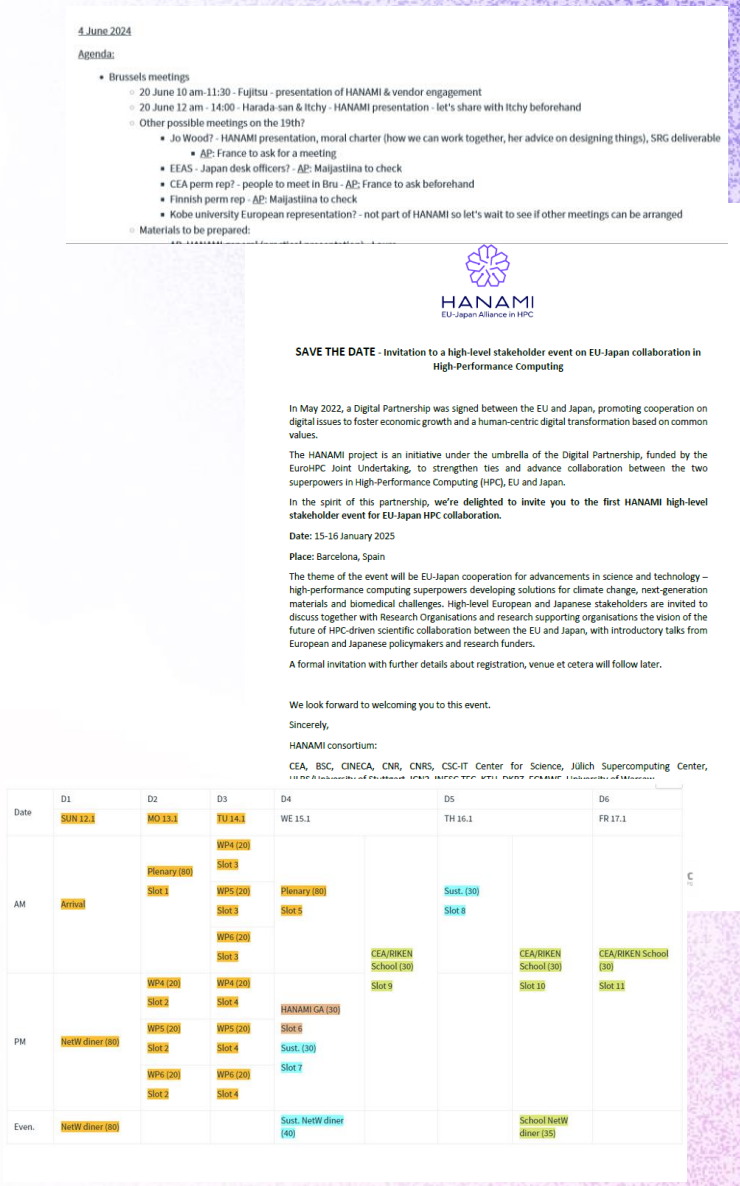
- Kickoff event in April 2024
- Session on HANAMI sustainability – questions discussed:
  - To the HANAMI consortium : **Do you agree with the key requirements for sustaining the collaboration? Is something missing?**
  - To wider audience : **What are the most efficient ways to ensure these requirements are fulfilled by the end of the project?**

WP7 The roadmap for sustainable Europe-Japan collaboration

- WP7 Roadshow in Brussels
  - Meeting with desk officers at EEAS to present HANAMI and invite them to the High-Level Symposium in January 2025
  - Meeting with senior executive of Fujitsu to introduce HANAMI and discuss possible collaborative efforts
  - Meeting with Science & Technology Councellor, Mission of Japan to the EU (MEXT) to present HANAMI
  - Discussion with Director of the European Office of RIKEN for insights on the Japanese policy landscape.

WP7 The roadmap for sustainable Europe-Japan collaboration

- Preparations for the WP7 sustainability event organized in conjunction of the Annual Symposium in January 2025
- Bi-monthly internal WP meetings
- Mapping of political decision makers and funders in the various consortium countries and in Japan in consultation with the Japanese collaborators (RIKEN)
- Planning for the engagement of policymakers and funders during HANAMI project (D7.1) in consultation with the Japanese collaborators (RIKEN)
- Detailed planning for the WP activities during the project in consultation with the Japanese collaborators (RIKEN) - ongoing



4 June 2024

Agenda:

- Brussels meetings
  - 20 June 10 am-11:30 - Fujitsu - presentation of HANAMI & vendor engagement
  - 20 June 12 am - 14:00 - Harada-san & Itchy - HANAMI presentation - let's share with Itchy beforehand
  - Other possible meetings on the 19th?
    - Jo Wood? - HANAMI presentation, moral charter (how we can work together, her advice on designing things), SRG deliverable
      - AP: France to ask for a meeting
    - EEAS - Japan desk officers? - AP: Maijastiina to check
    - CEA perm rep? - people to meet in Bru - AP: France to ask beforehand
    - Finnish perm rep - AP: Maijastiina to check
    - Kobe university European representation? - not part of HANAMI so let's wait to see if other meetings can be arranged
- Materials to be prepared:

HANAMI
EU-Japan Alliance in HPC

SAVE THE DATE - Invitation to a high-level stakeholder event on EU-Japan collaboration in High-Performance Computing

In May 2022, a Digital Partnership was signed between the EU and Japan, promoting cooperation on digital issues to foster economic growth and a human-centric digital transformation based on common values.

The HANAMI project is an initiative under the umbrella of the Digital Partnership, funded by the EuroHPC Joint Undertaking, to strengthen ties and advance collaboration between the two superpowers in High-Performance Computing (HPC), EU and Japan.

In the spirit of this partnership, **we're delighted to invite you to the first HANAMI high-level stakeholder event for EU-Japan HPC collaboration.**

Date: 15-16 January 2025

Place: Barcelona, Spain

The theme of the event will be EU-Japan cooperation for advancements in science and technology – high-performance computing superpowers developing solutions for climate change, next-generation materials and biomedical challenges. High-level European and Japanese stakeholders are invited to discuss together with Research Organisations and research supporting organisations the vision of the future of HPC-driven scientific collaboration between the EU and Japan, with introductory talks from European and Japanese policymakers and research funders.

A formal invitation with further details about registration, venue et cetera will follow later.

We look forward to welcoming you to this event.

Sincerely,

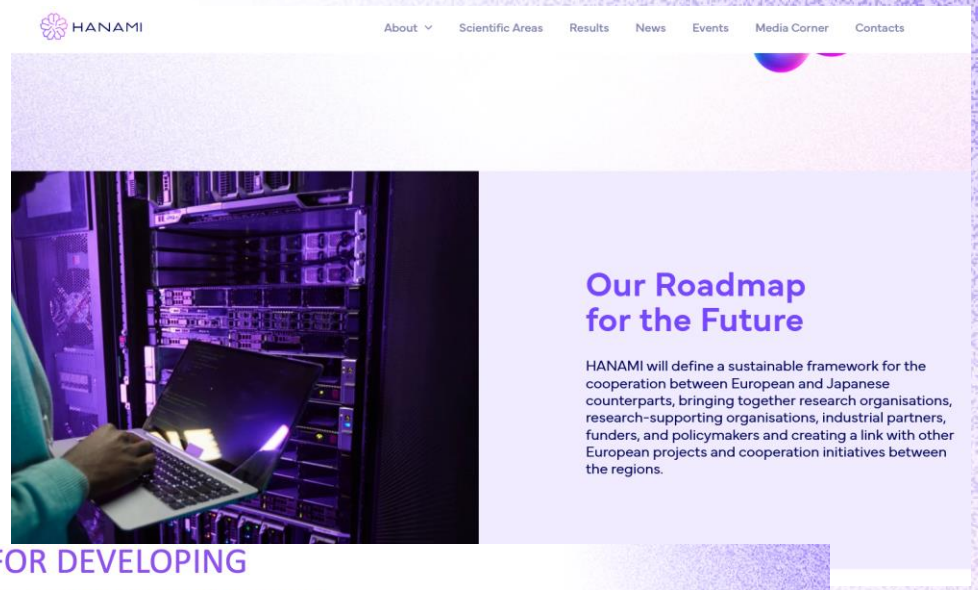
HANAMI consortium:

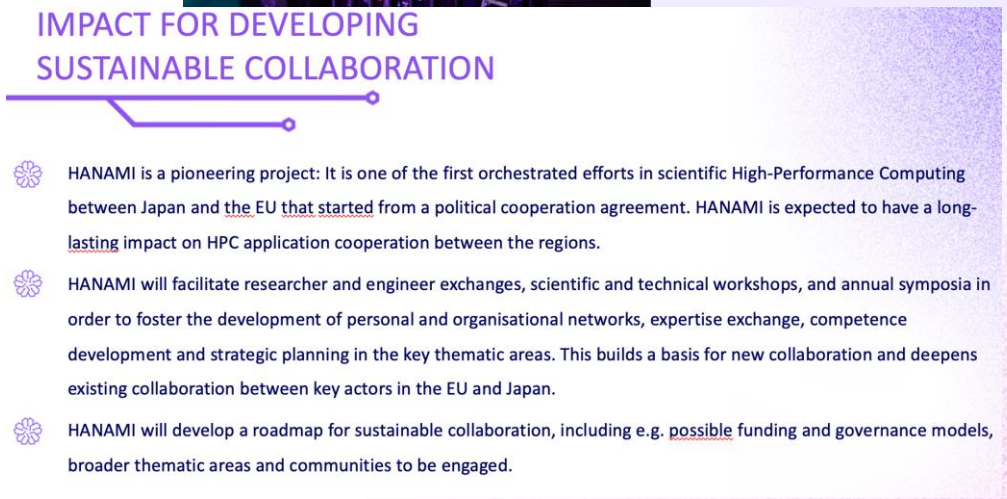
CEA, BSC, CINECA, CNR, CNRS, CSC-IT Center for Science, Jülich Supercomputing Center,

Date	D1	D2	D3	D4		D5		D6
	SUN 12.1	MO 13.1	TU 14.1	WE 15.1		TH 16.1		FR 17.1
AM	Arrival	Plenary (80) Slot 1	WP4 (20) Slot 3 WP5 (20) Slot 3 WP6 (20) Slot 3	Plenary (80) Slot 5	CEA/RIKEN School (30)	Sust. (30) Slot 8	CEA/RIKEN School (30)	CEA/RIKEN School (30)
PM	NetW diner (80)	WP4 (20) Slot 2 WP5 (20) Slot 2 WP6 (20) Slot 2	WP4 (20) Slot 4 WP5 (20) Slot 4 WP6 (20) Slot 4	HANAMI GA (30) Slot 6 Sust. (30) Slot 7	Slot 9		Slot 10	Slot 11
Even.	NetW diner (80)			Sust. NetW diner (40)			School NetW diner (35)	

WP7 The roadmap for sustainable Europe-Japan collaboration

- Sustainability work described on the website
  - Ongoing work
- Preparation of introduction material for presenting HANAMI to policymakers, funders and other stakeholders that are essential for the sustainability of the collaboration





WP7 The roadmap for sustainable Europe-Japan collaboration

Future plans:

- Organization of the first sustainability event in conjunction of the High-Level Symposium in Barcelona 01/2025
- Project internal workshop on impact assessment to support sustainability 10-11/2024
- Sustainability aspects contributed to possible HANAMI BoF in SC24 11/2024
- Continue development of network of policymakers, funders, and other key stakeholders for HANAMI sustainability (e.g. other related initiatives, industry, research organizations, etc.) - ongoing
- Bilateral discussions with national, EU and Japanese stakeholders on expectations towards HANAMI - ongoing (06/2024 - 12/2024)
- HANAMI travel grants used for an annual trip to Japan to meet policymakers, funders and other key stakeholders to understand their interests in HANAMI sustainability and promote HANAMI collaboration’s sustainability – first trip planned for 11-12/2024

WP3 Scientific and technology networking and community building

WP3 Scientific and technology networking and community building

- Key actions to foster technological and scientific networking between high-level European and Japanese researchers
  - strengthen and bring more visibility to existing collaborations and to strongly support the development of new collaborations with high added value

- WP3 objectives
  - Organize a yearly high-level workshop;
  - Promote long-term visits of European scientists and engineers in Japan, both within HANAMI core group but also on a larger scale;
  - Organize dedicated and specialized symposia, especially in collaboration with WP4-6 and the relevant European CoE in HPC

WP3 Scientific and technology networking and community building

Work package leader

Edouard Audit

HANAMI members

CSC

JÜLICH Forschungszentrum

BSC Barcelona Supercomputing Center Centro Nacional de Supercomputación

CINECA

HANAMI participants

RIKEN

WP3 Scientific and technology networking and community building

Fabrizio Gagliardi

Edouard Audit

Maijastiina Arvola

T3.1: Organisation of a yearly high-level symposium

WP3 Scientific and technology networking and community building

Edouard Audit

Fabrizio Gagliardi

Maijastiina Arvola

T3.2: Organisation of visits and extended stays to Japan

WP3 Scientific and technology networking and community building

Edouard Audit

Fabrizio Gagliardi

Maijastiina Arvola

Fabio Affinito

Edoardo Di Napoli

T3.3: Organization of scientific workshops

WP3 Scientific and technology networking and community building

T3.1 - Organisation of a yearly high-level symposium		
M1 01.03.2024 until M36 27.02.2027	  	• Manage the organization of a yearly high-level symposium gathering high-level scientists and engineers from Europe and Japan. • HANAMI Symposia will have three topical tracks corresponding to WP4-6 as well as a traversal HPC track. • Scientific and networking events and will allow promoting and strengthening existing collaborations and also fostering the birth of new fruitful collaborations. • Participants from core HANAMI partners, but also from other research organizations as well as industrials from Europe and Japan. The symposium will be managed by BSC in 2024, CEA in 2025 and CSC in 2026

M3.1	Events organised (marketing and communications conducted before and after)	M12 – 03.2025
R3.1	Report about the implementation high level symposia and travel grants use	M12 – 03.2025

WP3 Scientific and technology networking and community building

T3.2 - Organisation of visits and extended stays to Japan		
M1 01.03.2024 until M36 27.02.2027	  	• Promote and support visits and stays of European scientists and engineers to Japan, through travel grants • Committee responsible for evaluating applications and allocating these grants

M3.2	Events organised (marketing and communications conducted before and after)	M24 – 03.2026
R3.2	Report about the implementation high level symposia and travel grants use	M24 – 03.2026

WP3 Scientific and technology networking and community building

T3.3 - Organization of scientific workshops		
M1 01.03.2024 until M36 27.02.2027	 	• Organizing and hosting workshops to gather HANAMI and external partners around areas of interest (climate, material and biomedical). • The researchers will send their proposal to the WP3 committee, and according to the requests and rules established within HANAMI, the workshop request will be accepted.

M3.3	Events organised (marketing and communications conducted before and after)	M36 – 02.2027
R3.3	Report about the implementation high level symposia and travel grants use	M36 – 02.2027

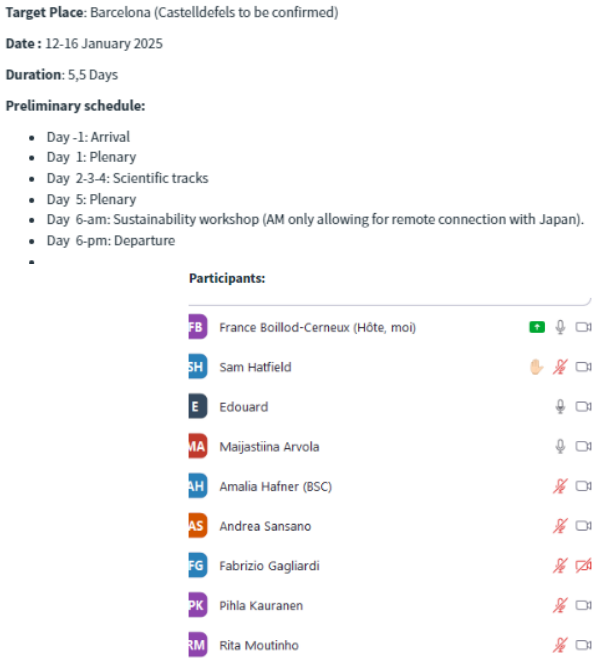
WP3 Scientific and technology networking and community building

- Travelling grants allocated for one year
  - WP2 to WP7 have received their travelling grants authorization
  - Each WP is now managing their visit organization. Reports and progress are shared through the regular Steering Boards.
  - Help and support from Project Coordinator and Project Manager to find fundings to invite the Japanese researchers for short and medium term visits in EU

France Boillod-Cerneux

Laure Caruso

WP3 Scientific and technology networking and community building



Target Place: Barcelona (Castelldefels to be confirmed)

Date : 12-16 January 2025

Duration: 5,5 Days

Preliminary schedule:

- Day -1: Arrival
- Day 1: Plenary
- Day 2-3-4: Scientific tracks
- Day 5: Plenary
- Day 6-am: Sustainability workshop (AM only allowing for remote connection with Japan).
- Day 6-pm: Departure

Participants:

- France Boillod-Cerneux (Hôte, moi)
- Sam Hatfield
- Edouard
- Maijastiina Arvola
- Amalia Hafner (BSC)
- Andrea Sansano
- Fabrizio Gagliardi
- Pihla Kauranen
- Rita Moutinho

- Regular meetings for High level Symposia event
  - Weekly meetings
  - Codesign of the event with Japanese consortium
    - Presence of Japanese consortium leader at each meeting (Kengo Nakajima, RIKEN/R-CCS)
  - Japanese Keynote speakers proposed for the event
    - About 8 Japanese Keynote speakers
  - Japanese participation within scientific work packages and sustainability event
    - Ongoing work

WP3 Scientific and technology networking and community building

- Leverage
  - Action in progress: Co-hosting of CEA/RIKEN school during HANAMI High level symposia
    - School on Kokkos framework
    - Focus on portability
  - Jointly defined by the CEA and RIKEN/R-CCS, the agenda is shared through HANAMI for completion if asked and possible. HANAMI students are welcomed within the CEA/RIKEN school.
  - Organizing committee

Miwako Tsuji

Kento Sato

Edouard Audit

France Boillod-Cerneux

WP4
Application development for the climate and weather modelling community

WP4 objectives and presentation

HANAMI

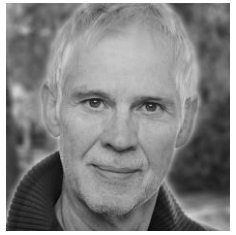
WP4 Application development for the climate and weather modeling community

- Connect Japanese and European efforts and expertise to improve the performance of codes for weather and climate simulations
  - 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

WP4 Application development for the climate and weather modelling community

Work package leaders

Joachim Biercamp



Mario Acosta

HANAMI members

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

DKRZ
DEUTSCHES KLIMARECHENZENTRUM

CSC

ECMWF

UNIVERSITY OF WARSAW

HANAMI participants

RIKEN

EVIDEN

東京大学 先端科学技術研究センター
Research Center for Advanced Science and Technology
The University of Tokyo

National Institute for Environmental Studies

WP4 July 2024 monthly meeting
Japanese and European partners together

WP4 Application development for the climate and weather modelling community

- Project 1: Replicability and skill of earth system models - Workflow and Interface
  - Task 4.1: Model assessment for earth system models and the integration through the workflow manager Autosubmit
- Project 2: Optimize, port and test European and Japan weather and climate codes
  - Task 4.2: High-Performance Climate and Weather benchmark
  - Task 4.3: The University of Warsaw Lagrangian Cloud Model (UWLCM)

WP4 Application development for the climate and weather modelling community – **research team**

Mario Acosta

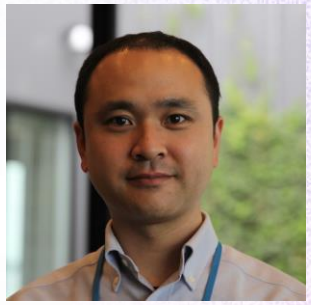
Kai Keller

Thomas Ludwig

Marta Alerany

Mohamed Wahib (Riken, JP)

Leo Arriola



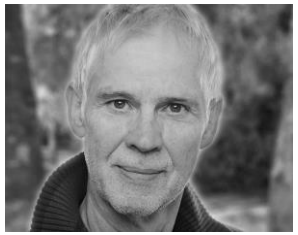
Hisashi Yashiro

T4.1: Model assessment for earth system models and the integration through the workflow manager Autosubmit

WP4 Application development for the climate and weather modelling community – **research team**

Chihiro Kodama

Hisashi Yashiro



Joachim Biercamp

Miguel Castrillo

Leopekka Saraste

Juhana Lankinen

Peter Duben

Samuel Hatfield

Erwan Raffin

T4.2: High-Performance Climate and Weather benchmark

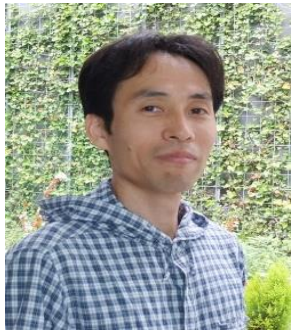
WP4 Application development for the climate and weather modelling community – **research team**

Hanna Pawlowska

Piotr Dziekan

Sin-Ichiro Shima

Seiya Nishizawa



Hirofumi Tomita

T4.3: The University of Warsaw Lagrangian Cloud Model (UWLCM)

WP4 ongoing actions

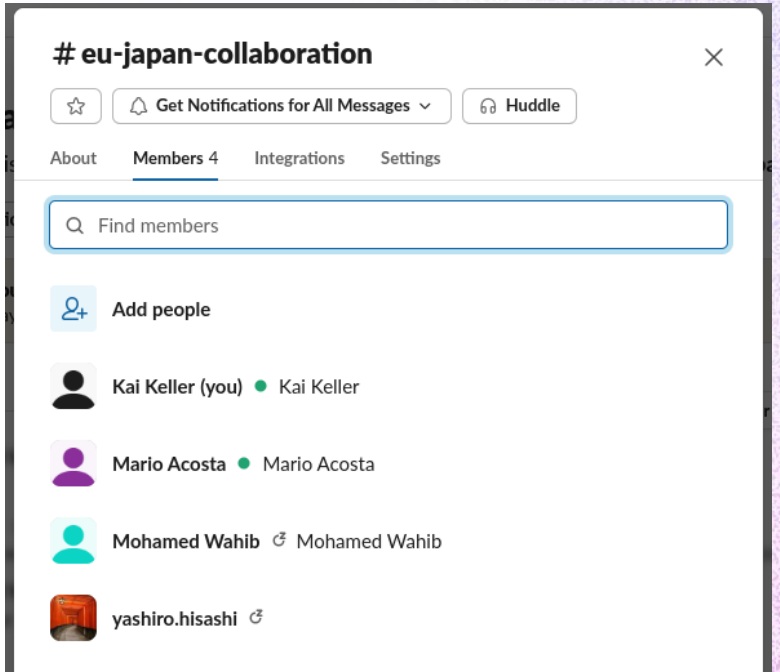
WP4 T4.1 Replicability and skill of earth system models - Workflow and Interface

T4.1 - Model assessment for earth system models and the integration through the workflow manager Autosubmit		
M3 01.05.2024 until M33 01.11.2026	BSC	develop the model assessment workflow addressing the requirements of ESMs from the European and Japanese partners
		deploy Autosubmit and the proposed workflow on Marenostrum 5, LUMI, and Fugaku.
	DKRZ DEUTSCHES KLIMARECHENZENTRUM	Developing the ESM replicability and model quality assessment aspects of the workflow
	RIKEN	Porting Japanese models to the workflow and assessing their replicability, projection skill, and performance on heterogeneous architectures

M4.1	Several collaborative interactions in place (workshops and meetings)	M06 - 06.2024
R4.1	Autosubmit workflow on Marenostrum5, LUMI and Fugaku (interim version)	M18 – 08.2025
R4.2	Autosubmit workflow on Marenostrum5, LUMI and Fugaku (final version)	M33 – 12.2026

WP4 T4.1 Replicability and skill of earth system models - Workflow and Interface

- Monthly meetings with Japanese researchers
  - 4 HANAMI members and 2 Japanese researchers attending the meetings
  - Quick communication using slack
  - Preparing internship of Leo Arriola to NIES under supervision of Hisashi Yashiro



WP4 T4.1 Replicability and skill of earth system models - Workflow and Interface

- Supercomputers access
  - Access granted for WP4P1 European team to Fugaku through HPCI access – duration: 05.2024 until 04.2025
    - Maximum of computing hours: 40000 nh
  - 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

WP4 T4.1 Replicability and skill of earth system models - Workflow and Interface

- Leverage
  - JST ASPIRE Call proposal – submitted on 08.2023
    - PI: Mohamed Wahib, RIKEN/R-CCS
    - Letter of support from HANAMI
    - Proposal rejected

  - JST ASPIRE Call proposal – submitted on 04.2024
    - PI: Mohamed Wahib, RIKEN/R-CCS
    - Letter of support from HANAMI and ESiWACE3
    - Proposal under review. Next step: November 2024.

WP4 T4.1 Replicability and skill of earth system models - Workflow and Interface

- Future plans
  - HANAMI travelling grant requested on 06.2024
    - Visit from researcher planned in 2024, 2025 and 2026.
    - Visited laboratory: Riken headquarters
  - Codes
    - Discussing the code portability on Fugakusupercomputer
    - Expecting starting date to port the code: 09.2024

WP4 T4.2: Optimize, port and test European and Japan weather and climate codes

WP4 T4.2 Optimize, port and test European and Japan weather and climate codes

T4.2 - High-Performance Climate and Weather benchmark		
M3 01.05.2024 until M33 01.11.2026	DKRZ	Contribute to maintenance, enhancement, document and testing of the framework; will foster dissemination and will track, collect and publish the results. It will support the implementation of ICON related components of HPCW on FUGAKU.
	BSC	Implement extensions of the HPCW on MN5, will support the implementation of Japanese components (in particular NICAM) on MN5 and support implementation of HPCW components on FUGAKU.
	ECMWF	Implement extensions of the HPCW on its own systems, maintain ECMWF-specific HPCW components. and support implementation of IFS related HPCW components on FUGAKU.
	CSC	Implement HPCW on LUMI, will contribute to its technical improvement and will support the implementation of Japanese components (in particular NICAM) on LUMI.

M4.1	Several collaborative interactions in place (workshops and meetings)	M06 - 06.2024
R4.3	Report on detailed work plan for extension of HPCW Report on extensions made to the HPCW benchmarks including results and conclusions	M18 – 08.2025
R4.4	Report on detailed work plan for extension of HPCW Report on extensions made to the HPCW benchmarks including results and conclusions	M33 – 12.2026

WP4 T4.2 Optimize, port and test European and Japan weather and climate codes

- Monthly WP4-wide meetings (including Japanese partners)
- Coordination with Japanese partners on Japanese HPCW components via email (e.g. NICAM)
- Personal Meeting of Mario and Joachim with Hisashi Yashiro at HPC workshop of ESiWACE CoE in May 2024 in Lecce to discuss HPCW aspects

WP4 T4.2 Optimize, port and test European and Japan weather and climate codes

- Supercomputers access (under negociation)
  - Access for WP4P2 European team to Fugaku through HPCI access – duration: 05.2024 until 04.2025
    - Maximum of computing hours: 40000 nh
  - Access for WP4P2 European team and Japanese collaborators to LUMI – duration: 05.2024 until 05.2025
    - Maximum of computing hours: 10 000 GPUh & 10 000 CPUh

WP4 P2 Optimize, port and test European and Japan weather and climate codes

- Future plans
  - 2-4 week trip to R-CCS (Kobe, Japan) for Samuel Hatfield and Niclas Schroeter under discussion
  - 2 week trip to R-CCS (Kobe, Japan) for Leopekka Saraste under discussion
    - Hosting a workshop
    - Discussing key elements in application porting tasks between LUMI and Fugaku
  - Codes
    - Discussing the code portability on Fugaku supercomputer
    - Effective work starting in 2025

WP4 T4.3 Optimize, port and test European and Japan weather and climate codes

T4.3 - The University of Warsaw Lagrangian Cloud Model		
M3 01.05.2024 until M33 01.11.2026	UNIVERSITY OF WARSAW	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 heterogeneus 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
	RIKEN	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.

M4.1	Several collaborative interactions in place (workshops and meetings)	M06 - 06.2024
R4.5	The scope of this deliverable will be to report activities for UWLCM	M33 – 12.2026

WP4P2 Optimize, port and test European and Japan weather and climate codes

- Monthly meetings with Japanese researchers
  - Regular exchanges on ICON
  - UWLCM: exchanges and information on framework
- Meeting with Japanese partners during International Cloud Modeling Workshop 2024 and International Conference on Clouds and Precipitation 2024

WP4 P2 Optimize, port and test European and Japan weather and climate codes

- Supercomputers access
    - Asked for LUMI and FUGAKU access via the HANAMI call

WP4 P2 Optimize, port and test European and Japan weather and climate codes

- Codes WP4P2

Codes	Supercomputer	Stage
UWLCM	Cyfronet Helios	Benchmark
	Fugaku	Start
	LUMI	Start

WP4P2 Optimize, port and test European and Japan weather and climate codes

- Leverage (in conjunction with WP4-P1)
  - JST ASPIRE Call proposal – submitted on 08.2023
    - PI: Mohamed Wahib, RIKEN/R-CCS
    - Letter of support from HANAMI
    - Proposal rejected
  - JST ASPIRE Call proposal – submitted on 04.2024
    - PI: Mohamed Wahib, RIKEN/R-CCS
    - Letter of support from HANAMI and ESiWACE3
    - Proposal under review. Next step: November 2024.

WP4P2 Optimize, port and test European and Japan weather and climate codes

- Future plans
  - HANAMI travelling grant requested on 07.2024, 2 weeks
    - Visit from researchers planned in 2025/2026
    - Visited laboratory: University of Hyogo, Kobe, Japan

WP5
Biomedical application co-development to address societal challenges

WP5 objectives and presentation

WP5 Biomedical application co-development to address societal challenges

- Advancing molecular life sciences computing by joint development of Exascale-focused algorithms
  - major simulation codes developed both in EuroHPC (GROMACS) and at RIKEN (GENESIS),
  - fast-multipole electrostatics,
  - bridging simulations and AI by implementing support for neural network-based nonbonded potentials.

- 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 modeling 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 tumor 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

WP5 Biomedical application co-development to address societal challenges

Work package leaders

Erik Lindahl

Alfonso Valencia

HANAMI members

KTH VETENSKAP OCH KONST

BSC Barcelona Supercomputing Center Centro Nacional de Supercomputación

CSC

JÜLICH Forschungszentrum

HANAMI participants

RIKEN

R-CCS

RIKEN BDR

東京工業大学 Tokyo Institute of Technology

九州大学 KYUSHU UNIVERSITY

東京大学 THE UNIVERSITY OF TOKYO

NAGOYA UNIVERSITY

university of groningen

Kobe University Graduate School of System Informatics
Kobe University Department of Computer Science and Systems Engineering

東京大学 先端科学技術研究センター
Research Center for Advanced Science and Technology
The University of Tokyo

WP5 Biomedical application co-development to address societal challenges

- WP5 – P1: Exascale electrostatics & machine learning to enable molecular dynamics of cell-size systems
  - Extend 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),
  - 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
    - unique codesign opportunity for both the European and Japanese

WP5 Biomedical application co-development to address societal challenges

- WP5 – P2: Development of genome analysis pipelines for Personalized Medicine
  - Provide mechanistic models for individual patients reflecting their differential genomic composition and response to treatments
  - Interpret mechanistic models with field-experts to identify potential treatments and/or associated signatures
  - Contribute 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

WP5 Biomedical application co-development to address societal challenges

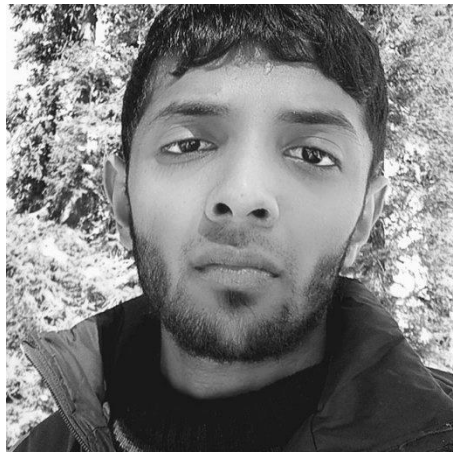
- WP5 – P3: Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses
  - Develop a pipeline for AI-assisted automated large-scale computational fluid dynamics (CFD) simulations to analyze respiratory diseases
  - Use AI-methods to accelerate CFD simulations
  - Provide an AI-assisted automated surgery tool to surgeons as a demonstrator
  - Develop a tool for assessing the risk of exhaled infectious (virus) in indoor scenarios
  - All implementations complement missing elements in either the m-AIA (EU) or the CUBE (Japan) CFD solvers
  - AI methods are jointly developed with the Japanese partners

WP5 Biomedical application co-development to address societal challenges – **research team**

Prof. Berk Hess

Szilárd Páll

Dr. Muhammad Sadiq



Prof. Erik Lindahl

Assoc. Prof Rio Yokota

T5.1: ExaFMM - solving the scaling problem for electrostatic interactions

WP5 Biomedical application co-development to address societal challenges – **research team**

Prof. Erik Lindahl

Prof. Berk Hess

Prof. Yuji Sugita

Prof. Makoto Taiji

Dr. Alessandra Villa

Dr. Muhammad Sadiq

Dr. Mohamad Wahib

Prof. Florence Tama

T5.2: Data-driven biomolecular modeling & simulation

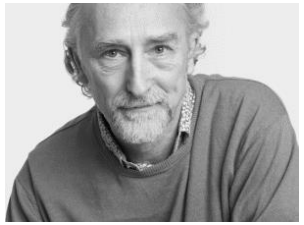
WP5 Biomedical application co-development to address societal challenges – **research team**

Tommi Nyrönen

Julio Saez-Rodriguez

David Torrents

Professor Okada Mariko



Alfonso Valencia

Professor
Hiroyuki Aburatani

Professor Mikita Suyama

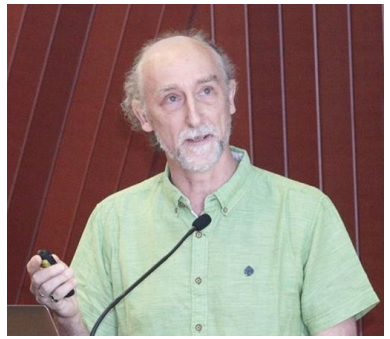
Shinya Kuroda

Emmanuel Barillot

Reinhard Schneider

T5.3: Genome analysis pipeline

WP5 Biomedical application co-development to address societal challenges – **research team**

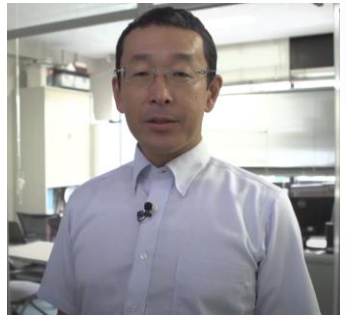


Alfonso Valencia

Tommi Nyrönen

EU Japan

Elisa Domínguez-Hüttinger
(PRIMe - Osaka University)



Shinya Kuroda
(University of Tokyo)

Mariko Okada
(Osaka University)

T5.4: Tumour evolution simulation pipelines

WP5 Biomedical application co-development to address societal challenges – **research team**

Andreas Lintermann

Prof. Wolfgang Schröder

Prof. Makoto Tsubokura

T5.5: AI-assisted automated CFD pipelines and acceleration of CFD computations
T 5.6: AI-assisted surgery planning and risk assessment of exhaled infectious aerosols

WP5 ongoing actions

WP5P1 Exascale electrostatics & machine learning to enable molecular dynamics of cell-size systems

WP5P1 Exascale electrostatics & machine learning to enable molecular dynamics of cell-size systems

T5.1 - ExaFMM - solving the scaling problem for electrostatic interactions		
M1 01.03.2024 until M36 27.02.2027		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.

M5.1	Several collaborative interactions in place such as visits and exchanges	M18 – 08.2025
R5.1	Biomedical project setup roadmap	M06 - 06.2024

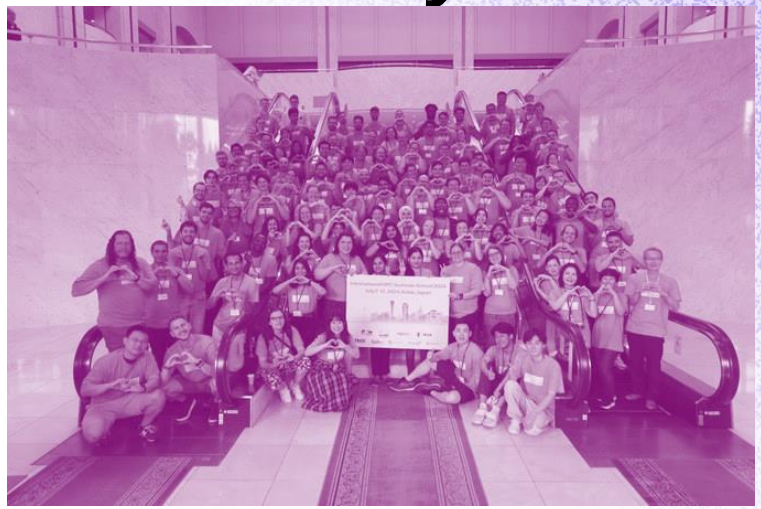
WP5P1 Exascale electrostatics & machine learning to enable molecular dynamics of cell-size systems

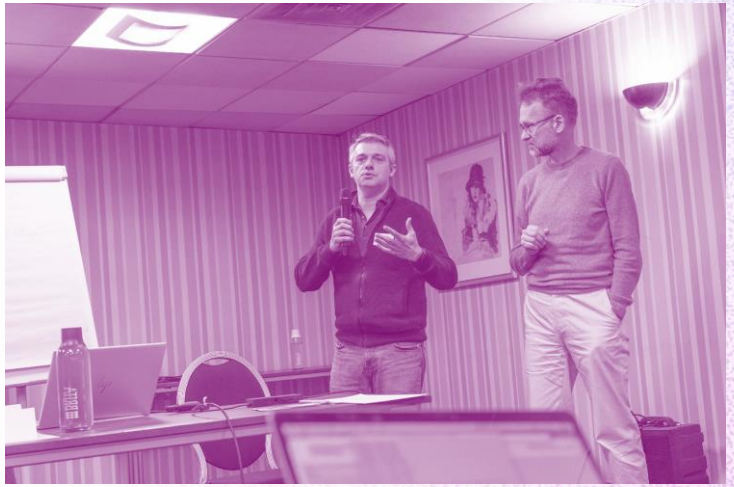
T5.2 - Data-driven biomolecular modeling & simulation		
M1 01.03.2024 until M36 27.02.2027	KTH, R-CCS, RIKEN BDR	work on improving the support for neural network/deep learning potentials by integrating DeepMD and other packages into both GROMACS and GENESIS, Evaluate the possibility of directly implementing code to do the inference stage
	KTH, R-CCS, RIKEN BDR	Address the challenges with sensitivity to training domains, Investigate possibilities to use “delta-learning”, Apply neural networks as a correction
	KTH, R-CCS, Nagoya University, RIKEN BDR, Oxford	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 modeling of cellscale systems restrained with low-resolution experimental data

M5.1	Several collaborative interactions in place such as visits and exchanges	M18 – 08.2025
R5.2	Biomedical halftime report	M18 – 08.2025

WP5P1 Exascale electrostatics & machine learning to enable molecular dynamics of cell-size systems

- Regular meetings with Japanese researchers
  - Long-range electrostatics work has started, new postdoctoral scholar recruited on EuroHPC side
  - Regular exchanges on zoom
  - Extensive RIKEN contributions to GROMACS SVE acceleration and regression testing on Fugaku hardware
  - Joint Exascale-target fast multipole implementation has started with Prof. Rio Yokota, first targeting GROMACS.
- RIKEN-CCS GENESIS team has become involved in definitions of joint file formats and data exchange standards run by the EU teams





WP5P1 Exascale electrostatics & machine learning to enable molecular dynamics of cell-size systems

- First collaborative visit, research presentation and mini-workshop by Erik Lindahl in Kobe July 2024, in conjunction with IHPCSS Summer school.
- Additional planned research visits:
  - Dr. Muhammad Sadiq to visit Tokyo Tech late 2024 for joint ExaFMM work
  - Prof. Berk Hess visit to RIKEN & Tokyo Tech planned mid-to-late 2025 to finalize work
  - 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
- New AI4SCIENCE frameworks both in Sweden & Japan to focus on data-driven work and foundation models. Will pursue new collaborations with Profs. Yuji Sugita & Satoshi Matsuoka.

WP5P1 Exascale electrostatics & machine learning to enable molecular dynamics of cell-size systems

- Codes WP5P1

Codes	Supercomputer	Stage
GROMACS	MARENOSTRUM 5, MELUXINA, KAROLINA, DISCOVERER, VEGA, DEUCALION, LEONARDO	Production, fully optimized.
	LUMI	Production, further HIP-specific optimization in progress
	Fugaku	Production, further SVE-specific optimization in progress
	JUPITER, JULES VERNE	Production will be supported day 1. New SVE-optimization in progress based on Fugaku work.

WP5P2 Development of genome analysis pipelines for Personalized Medicine

WP5P2 Development of genome analysis pipelines for Personalized Medicine

T5.3 - Genome analysis pipeline		
M1 01.03.2024 until M36 27.02.2027		genome analysis pipeline with variants for different type of genomic data
		use different type of genomic and clinical information including real data complemented with generated synthetic data
		modelling of the cohorts of synthetic data between the participating labs in Japan and Europe
		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.

M5.1	Several collaborative interactions in place such as visits and exchanges	M18 – 08.2025
R5.3	Biomedical final results	M36 – 02.2027

WP5P2 Development of genome analysis pipelines for Personalized Medicine

T5.4 - Tumour evolution simulation pipelines		
M1 01.03.2024 until M36 27.02.2027		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.
		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
		produce pipelines that can be executed by non-experts without the need of further adaptations beside setting the input data and basic parameters

M5.1	Several collaborative interactions in place such as visits and exchanges	M18 – 08.2025
R5.4	Final report on scientific progress in molecular life science and personalized medicine, as well as updated long-term collaboration roadmap	M36 - 02.2027

WP5P2 Development of genome analysis pipelines for Personalized Medicine

- Monthly meetings with Japanese researchers
  - Evaluate synthetic data generation pipelines
    - How to integrate somatic alterations from real patients to improve synthetic data quality
    - Potential applications in Personalised Medicine and computational biology
  - Plan research visits
  - Coordinately organise workshops on HPC-simulations in biology
  - Explore opportunities for joint publications
  - Organise inter-center working teams

Alfonso Valencia (BSC)

Tommi Nyrönen (CSC)

Shinya Kuroda (University of Tokyo)

Mariko Okada (Osaka University)

Elisa Domínguez-Hüttinger (PRIMe - Osaka University)

WP5P2 Development of genome analysis pipelines for Personalized Medicine

- Monthly meetings with Japanese researchers
  - Identify grand challenges in Personalised Medicine requiring exascale capacities
    - Large-scale prediction of combinatorial drug treatments
    - Explore landscape of attractors in super complex molecular pathways
    - Integration of genome-scale metabolic networks in cellular simulations
    - Hero runs: From molecular features to whole organ simulations

Alfonso Valencia (BSC)

Tommi Nyrönen (CSC)

Shinya Kuroda (University of Tokyo)

Mariko Okada (Osaka University)

Elisa Domínguez-Hüttinger (PRIMe - Osaka University)

WP5P2 Development of genome analysis pipelines for Personalized Medicine

- Coordinate efforts for computationally benchmarking of genomic pipelines in European + Japanese HPC facilities
  - Comparative test in MN5-LUMI vs Fugaku
  - Evaluate parallel and distributed computing efficiency on…
    - Synthetic data generation pipelines
    - Tumour evolution multiscale simulations
  - Metrics
    - CPU time, memory consumption or I/O
    - Parallel and communication efficiency and computational scalability
    - Energy metrics

Alfonso Valencia (BSC)

Tommi Nyrönen (CSC)

Elisa Domínguez-Hüttinger (PRIMe - Osaka University)

WP5P3 Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses

WP5P3 Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses

T5.5 - AI-assisted automated CFD pipelines and acceleration of CFD computations		
M1 01.03.2024 until M6 31.08.2024	JÜLICH Forschungszentrum	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 flow through a randomly constricted 90 degree elbow pipe
	JÜLICH For RIKEN KOBE UNIVERSITY	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
	RIKEN KOBE UNIVERSITY	Employing deep learning techniques for flow field decomposition to investigate different modes of flow fields

M5.1	Several collaborative interactions in place such as visits and exchanges	M18 – 08.2025
R5.5	Intermediate report on scientific advancements in Personalized Medicine at the Macroscopic Level	M21 – 11.2025

WP5P3 Personalized Medicine on Macroscopic Level: Repiratory Flows and Infection Risk Analyses

T5.6 - AI-assisted surgery planning and risk assessment of exhaled infectious aerosols		
M1 01.03.2024 until M6 31.08.2024	JÜLICH Forschungszentrum 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
	JÜLICH Forschungszentrum	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
	RIKEN KOBE UNIVERSITY	Coupling CUBE simulations of indoor scenarios to a genetic algorithm to opitimize the interior design of clinical facilities

M5.1	Several collaborative interactions in place such as visits and exchanges	M18 – 08.2025
R5.6	Final report on scientific advancements in Personalized Medicine at Macroscopic Level	M36 – 02.2027

WP5P3 Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses

- Bi-weekly meetings with Japanese researchers to exchange progress of the Joint Laboratory for Extreme Scale Computing (JLESC) Project “Deep Neural Networks for CFD Simulations”
- Further online meetings to achieve the following:
  - Joint publication about physics-informed neural networks for flow predictions[1]
  - Joint publication about the decomposition of flow fields with machine learning[2]
  - 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[3,4]

[1] Rishabh Puri, Junya Onishi, Mario Rüttgers, Rakesh Sarma, **Makoto Tsubokura**, **Andreas Lintermann**: On the choice of physical constraints in artificial neural networks for predicting flow fields, Future Generation Computer Systems, Volume 161, 2024, doi:10.1016/j.future.2024.07.009.

[2] Aito Higashida, Kazuto Ando, Mario Rüttgers, **Andreas Lintermann**, **Makoto Tsubokura**: Robustness evaluation of large-scale machine learning-based reduced order models for reproducing flow fields, Future Generation Computer Systems, Volume 159, 2024: 10.1016/j.future.2024.05.005.

[3] Mario Rüttgers, Fabian Hübenthal, **Makoto Tsubokura**, **Andreas Lintermann**: Parallel reinforcement learning and Gaussian process regression for improved physics-based nasal surgery planning, accepted at AGCA workshop, PPAM conference, Ostrava, 2024.

[4] **Makoto Tsubokura**, Rahul Bale, Alicia Murga, Kazuhide Ito, Mario Rüttgers, **Andreas Lintermann**: HPC-CFD based optimization of indoor environment to minimize airborne containments, accepted at AGCA workshop, PPAM conference, Ostrava, 2024.

WP5P3 Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses

- Supercomputers access
  - Access granted for WP5, P3 Japanese researchers to JURECA-DC through the Gauss Centre for Supercomputing (GCS) compute project ”Improved Diagnostics of Respiratory Flows Using a Lattice-Boltzmann Method and Machine Learning Techniques” – duration: 05.2024 until 04.2025
    - Maximum of computing hours: 50,000 GPU-h, 50,000 CPU-h

WP5P3 Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses

- Codes WP5, P3

Codes	Supercomputer	Stage
m-AIA	JUWELS, JURECA-DC	Production
	Fugaku	Start
CUBE	Fugaku	Production
	JUWELS, JURECA-DC	Start

WP5P3 Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses

- Leverage
  - JST ASPIRE Call proposal – submitted on 08.2023
    - PI: Makoto Tsubokura, RIKEN/R-CCS
    - Letter of support from HANAMI
    - Proposal rejected
  - JST ASPIRE Call proposal – submitted on 04.2024
    - PI: Makoto Tsubokura, RIKEN/R-CCS
    - Letter of support from HANAMI
    - Proposal under review. Next step: November 2024.

WP5P3 Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses

- Future plans
  - HANAMI travelling grant requested on 07.2024, 2 weeks
    - Visit from researcher planned in 04.2025
    - Visited laboratory: Complex Phenomena Unified Simulation Research Team, Kobe, Japan
  - Codes
    - Discussing the portability of the m-AIA code on the Fugaku supercomputer
    - Running the developed tools on the Fugaku supercomputer
    - Effective work starting on 04.2025

WP6
HPC for future materials design

WP6 objectives and presentation

WP6 HPC for future materials design

- HPC to study and optimize various materials properties to develop sustainable energy technologies
- HPC enables new dimensions of materials design, increasing
  - complexity of the accessible systems and properties,
  - accuracy and improved approximations of the computational approaches
- Combination of HPC, high-throughput and materials informatics capacities,
  - Address major societal and technological challenges
- Strengthening the EUJapan collaboration
  - Improving materials sustainability in applications of relevance for energy production and storage
  - Joint development efforts for extremely scalable libraries and innovative software that may enable future frontier applications

WP6 HPC for future materials design

- Push the frontiers of in silico simulations of innovative materials for sustainable energy production and storage
- Share and advancing optimized codes developed in Europe and Japan
  - Interoperability and use on the most performing systems
- Develop numerical libraries capable of executing at scale
- Identify future challenges and opportunities for materials research in the evolving HPC ecosystem and in emerging technological trends

WP6 HPC for future materials design

Work package leaders

Edoardo Di Napoli

Elisa Molinari

HANAMI members

HANAMI participants

WP6 HPC for future materials design

- 2 projects within WP6
- WP6 – P1: Sustainable materials for photovoltaics and energy storage
- WP6 – P2: Exascale Materials Science simulations through extremely scalable libraries and innovative software

WP6 HPC for future materials design

M6.1	All HANAMI code, workflows and databases developed in project available in public repositories or servers.	M18 – 08.2025
M6.2	snapshot of the major codes involved in the WP in the form of code releases addressing the code improvements accessible in publicly available repository	M36 – 02.2027
R6.1	Report on the initial set up of the projects and the building and consolidating of the collaborations with the Japanese partners	M06 - 08.2024
R6.2	First projects results and outlook on sustainability of EU-Japan collaboration with indication of prospective enlargement of collaborative partnership	M18 – 08.2025
R6.3	Results of the projects and outlook on future activities.	M36 – 02.2027

WP6 HPC for future materials design – **research team**

Giacomo Giorgi

Takahito Nakajima

Koichi Yamashita

Daniele Varsano

Maurizia Palummo

T6.1: Sustainable materials for photovoltaics

WP6 HPC for future materials design – **research team**

Pablo Ordejon

Yoshitaka Tateyama

Minoru Otani

Deborah Prezzi

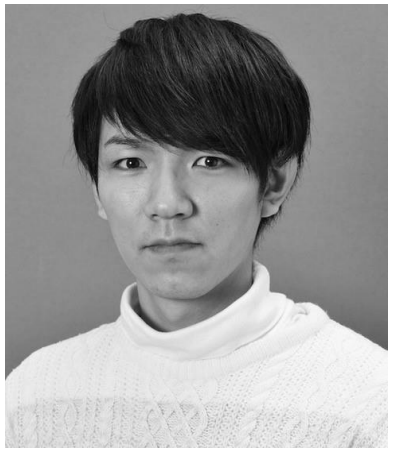
Stefan Blugel

T6.2: Electrochemistry and battery research from first principles

WP6 HPC for future materials design – **research team**

Michele Casula

Kosuke Nakano



Marco Cherubini

Abhishek Raghav

T6.3: Hydrogen storage: adsorption, desorption, reaction barriers from QMC

WP6 HPC for future materials design – **research team**

Edoardo Di Napoli

Toshiyuki Imamura

Luigi Genovese

Kengo Nagajima

William Dawson

Alessandro Pecchia

T6.4: Numerical linear algebra framework for Materials Science

WP6 HPC for future materials design – **research team**

Alessandro Pecchia

Takahito Nakajima

Tetsuya Sakurai

Taisuke Ozaki

Edoardo Di Napoli

Luigi Genovese

T6.5: Non-equilibrium charge-carrier dynamics in 2d-materials

WP6 HPC for future materials design – **research team**

Luigi Genovese

Takahito Nakajima

Sergeij Manzhos

Edoardo Di Napoli

Alessandro Pecchia

T6.6: Enhancing Materials Science scalability through innovative block sparse libraries

WP6 ongoing actions

WP6P1 Sustainable materials for photovoltaics and energy storage

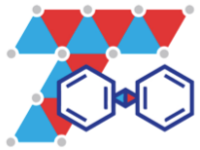
WP6P1 Sustainable materials for photovoltaics and energy storage

T6.1 - Sustainable materials for photovoltaics		
M1 01.03.2024 until M36 27.02.2027	National Research Council of Italy RIKEN 横浜市立大学 YOKOHAMA CITY UNIVERSITY 東京大学 THE UNIVERSITY OF TOKYO	Characterize more sustainable materials for perovskite-based solar cells (PSCs), in particular Pb-less and Pb-free PSCs. Calculate the interface and GBs from first-principles combining such calculations with large-scale quantum chemistry ones Simulation of GBs of realistic size (NTChem code), 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. Massive usage of HPC resources is mandatory to achieve our goals.

WP6P1 Sustainable materials for photovoltaics and energy storage

T6.2 - Electrochemistry and battery research from first principles		
M1 01.03.2024 until M36 27.02.2027	ICN2 National Research Council of Italy JÜLICH Forschungszentrum	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)
	NIMS 物質・材料研究機構	The EU team is expert in the development of DFT methods and their implementation on efficient codes (SIESTA)
	筑波大学 University of Tsukuba	Implement and optimize the code and demonstrate efficient and relevant calculations of the electrified interface.

WP6P1 Sustainable materials for photovoltaics and energy storage

T6.3 - Hydrogen storage: adsorption, desorption, reaction barriers from QMC		
M1 01.03.2024 until M36 27.02.2027	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**. Workflow manager: **TurboGenius**  TurboRVB

WP6P1 Sustainable materials for photovoltaics and energy storage

- Monthly meetings with Japanese researchers
  - 3 HANAMI members and 2 Japanese researchers attending the meetings
  - Regular exchanges on ESM
  - Yambo & SIESTA: exchanges and information on framework
  - TurboRVB: weekly zoom meetings + Kosuke Nakano (NIMS) visit to Paris (Sorbonne U, CNRS) planned early September 2024

WP6P1 Sustainable materials for photovoltaics and energy storage

- Supercomputers access
    - Access granted for WP6P1 European team to Fugaku:

Yambo Trial Access Project, project Yambo Scale: hp240326 through HPCI access

Duration: 09.2024 up to 6 months max.

Maximum of computing hours: 100000 nh

TurboRVB Regular Access Project, project number hp240033 through HPCI access

Duration: FY2024 (01.04.2024 - 31.03.2025)

Maximum of computing hours: 5M nh

WP6P1 Sustainable materials for photovoltaics and energy storage

- Supercomputers access
    - Access granted to French supercomputers:

TurboRVB Regular Access Project, project number A0150906493 through GENCI access

Duration: 01.11.2023 - 31.10.2024 (to be renewed this year for 2025)

Maximum of computing hours: Rome TGCC (6M core hours), SkyLake TGCC (1M core hours), Jean-Zay IDRIS GPU partition (1M GPU hours), Jean-Zay IDRIS CPU partition (2M CPU hours)

GENCI
HPC at the service of knowledge

TGCC
Très Grand Centre de calcul du CEA

idris

WP6P1 Sustainable materials for photovoltaics and energy storage

- Codes WP6P1

Codes	Supercomputer	Stage
Quantum ESPRESSO	ECMWF-ATOS	Production
	LUMI	Benchmark
	DKRZ-Levante	Development
	Fugaku	Start

WP6P1 Sustainable materials for photovoltaics and energy storage

- Codes WP6P1

Codes	Supercomputer	Stage
Yambo	Fugaku	Benchmark
TurboRVB	Fugaku	Production
TurboGenius	Fugaku	Development/Production
TurboGenius	TGCC (CEA)	Development/Benchmark

WP6P1 Sustainable materials for photovoltaics and energy storage

- Leverage
  - Extreme scale access EuroHPC proposal – submitted on 04.2024
    - PI: Michele Casula, CNRS
    - HANAMI project at the core of the proposal
    - Proposal under review

WP6P1 Sustainable materials for photovoltaics and energy storage

- Future plans
  - HANAMI travelling grant requested on 06.2024
    - Visit from researcher (Giorgi, Varsano, Post-doc) planned in 06-07.2025, 2-4 weeks; visited laboratory: Yamashita Lab, Yokohama, Japan.
    - Visit of CNRS team (Casula, Raghav, Cherubini) planned in 04.2025, 2 weeks; visited laboratory: NIMS, Tsukuba, Japan.
  - Yambo
    - Discussing the code portability on Fugaku supercomputer
    - Expecting starting date to port the code: 12.2024
  - TurboRVB
    - Portability of workflow manager TurboGenius across different (European and Japanese) HPC platforms

WP6P1 Sustainable materials for photovoltaics and energy storage

- Future plans
  - Workshop
    - Workshop organization around WP6 topics involving both European and Japanese community

WP6P2 Exascale Materials Science simulations through extremely scalable libraries and innovative software

WP6P2 Exascale Materials Science simulations through extremely scalable libraries and innovative software

T6.4 - Numerical linear algebra framework for Materials Science		
M1 01.03.2024 until M36 27.02.2027	JÜLICH Forschungszentrum RIKEN cea National Research Council of Italy 東京大学 THE UNIVERSITY OF TOKYO	Standard framework for large-scale numerical linear algebra libraries development Provides a common platform for developers and users to access and utilize various numerical libraries and data structures Promotes interoperability and collaboration among the different supercomputing centersand research groups making up the EU-Japan landscape; Enables researchers to easily benchmark and evaluate the performance of different parallel algorithms

WP6P2 Exascale Materials Science simulations through extremely scalable libraries and innovative software

T6.5 - Non-equilibrium charge-carrier dynamics in 2d-materials	
M1 01.03.2024	Development of parallelNEGF & interfacing BigDFT Massively parallel solver with electron-phonon and electron-photon interactions
until	Implement a framework for the representation of block sparse (with dense blocks) data operating close to peak memory bandwidth and tailored to accelerated platforms.
M36 27.02.202	Integrate both data framework and abstraction interface in MS code such as BigDFT and ibNEGF.

WP6P2 Exascale Materials Science simulations through extremely scalable libraries and innovative software

T6.6 - Enhancing Materials Science scalability through innovative block sparse libraries		
M1 01.03.2024 until M36 27.02.2027	cea	Extend the scaling fo BigDFT by progressively combining the current features of the code with ongoing developments in tasks 6.4
	RIKEN	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
	National Research Council of Italy JÜLICH Forschungszentrum	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.

WP6P2 Exascale Materials Science simulations through extremely scalable libraries and innovative software

- Regular meetings with Japanese researchers
  - Monthly exchanges 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.

slack

GitLab

WP6P2 Exascale Materials Science simulations through extremely scalable libraries and innovative software

- Workshop in Forschungszentrum Juelich, Germany – March 13-15, 2024
  Participants : FZJ and RIKEN-CCS

WP6P2 Exascale Materials Science simulations through extremely scalable libraries and innovative software

- Supercomputers access
  - Access granted for FZJ team to Fugaku through HPCI access – duration: 10.2023 until 09.2024
    - Maximum of computing hours: 3,200,000 node-h
  - Access granted to FZJ team to Wisteria through JHPCN – duration 05.2024 until 04.2025

  - Access to be granted for WP6P2 Japanese researchers to JUWELS and JUPITER through bilateral MoU FZJ and RIKEN/R-CCS

WP6P2 Exascale Materials Science simulations through extremely scalable libraries and innovative software

- Codes WP6P2

Codes	Supercomputer	Stage
ChASE	JUWELS Cluster and Booster	Production
	FUGAKU	Benchmark
	Wisteria	Benchmark
	Vega	Benchmark
	JEDI (JUPITER precursor)	Development

WP6P2 Exascale Materials Science simulations through extremely scalable libraries and innovative software

- Codes WP6P2

Codes	Supercomputer	Stage
libNEGF	JUWELS Cluster and Booster	Benchmark
	JEDI (JUPITER precursor)	Development
	FUGAKU	Start

WP6P2 Exascale Materials Science simulations through extremely scalable libraries and innovative software

- Codes WP6P2

Codes	Supercomputer	Stage
BigDFT	Fugaku	Production
	LUMI	Benchmark

WP6P2 Exascale Materials Science simulations through extremely scalable libraries and innovative software

- Leverage
  - JST ASPIRE Call proposal – submitted on 08.2023
    - PI: Takahito Nakajima, RIKEN/R-CCS
    - Letter of support from HANAMI
    - Proposal rejected
- Supporting call
  - Inno4Scale call projest ‘LimitX’— duration 02.2024 - 01.2025

WP6P2 Exascale Materials Science simulations through extremely scalable libraries and innovative software

- Future plans
  - HANAMI travelling grant requested on 06.2024, 8 weeks
    - Visit from researcher planned in 03.2025 and 03.2026
    - Visited laboratory: RIKEN-CCS, Kobe, Japan
  - Codes
    - Discussing the code integration and portability on Fugaku supercomputer and planning for the FUGAKU-NEXT project
    - Effective work starting on 01.2025

THANK YOU!

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Funded by the European Union

EuroHPC Joint Undertaking

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