HANAMI

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

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Intermediate report on scientific advancements in Personalized Medicine at the Macroscopic Level

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Executive Summary

This midterm deliverable specifically presents the progress of WP5 deliverable from Forschungszentrum Juelich, advancing personalised medicine through a combination of multiscale modelling and High-Performance Computing (HPC). At the physical scale of nasal cavity flows, AI-augmented computational fluid dynamics simulations of respiratory flow and viral transport are performed to improve the success of rhinology treatment as well as to assess patient-specific infection risks. These efforts form a unified framework that leverages international collaboration and HPC to enable predictive, personalised health modelling.

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1. Introduction

The HANAMI partner Juelich, more specifically the Simulation and Data Laboratory Fluids and Solids Engineering (SDL FSE) from the Jülich Supercomputing Centre (JSC) works in Work Package 5 (WP5) on two biomedical use cases (Tasks 5.5 and 5.6) that relate to the domain of Computational Fluid Dynamics (CFD). The investigations concentrate on analyses and simulations on a macroscopic level. They introduce physical models and corresponding simulation methods, such as the Lattice-Boltzmann method, on a microscopic level. The work is jointly performed with the Japanese partner from the RIKEN Center for Computational Science (R-CCS), i.e., Prof. Makoto Tsubokura, the head of the Complex Phenomena Unified Simulation Research Team and his colleagues at R-CCS. The simulations make use of the multi-physics open-source simulation code m-AIA[1], mainly developed by the Institute of Aerodynamics and Chair of Fluid Mechanics, RWTH Aachen University, and co-developed by Juelich. Furthermore, the group at R-CCS develops and uses the CUBE code, which is an R-CCS in-house closed-source code.

This deliverable reports on Project 3 “Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses” in WP5 and its activities in the corresponding tasks, i.e., Task 5.5 “AI-assisted automated CFD pipelines and acceleration of CFD computations” and Task 5.6 “AI-assisted surgery planning and risk assessment of exhaled infectious aerosols”.

This project aims to advance the current state of the art in personalised medicine by leveraging a combination of existing CFD methodologies, i.e., the Lattice-Boltzmann method implemented in the m-AIA code, and various rapidly evolving AI components. Specifically, this is done through two tasks, which define two related but distinct use cases in the field of respiratory flows.

Task 5.5 concerns accelerating and enhancing the various steps of CFD workflows for personalised medicine with the help of AI components. JSC brings its expertise in super-resolution techniques utilising convolutional neural networks for increasing the resolution of computer tomography data, as well as physics-informed neural networks for flow initialisation. These methodologies are applied to the problem of nasal cavity flows. The application of the super-resolution technique allows for increased fidelity of the simulation, as the numerical accuracy of the underlying nasal cavity geometry is less limited by the spatial resolution of CT imaging. Additionally, the total simulation time can be further shortened by using physics-informed neural networks (PINNs) for specifying an initial condition, which is closer to the converged state. Thus, fewer iterations of the solution process are required, leading to a reduction in the total computational time and effort.

The work in Task 5.6 further promotes the use of AI components and allows for an AI-assisted surgical geometry modification by utilising a reinforcement learning (RL) algorithm that suggests a modified nasal cavity geometry. This modified geometry is a solution to an

[1] m-AIA repository https://git.rwth-aachen.de/aia/m-AIA/m-AIA

optimisation problem, where the pressure loss and temperature difference are used simultaneously as objective functions. This physics-driven modification potentially improves the overall comfort of the patient. The optimisation problem can be further extended to also account for other objective functions, such as balanced volume flow rate through both nasal passages and surface wall-shear stress.

These two tasks primarily build on the existing experience of the SDL FSE with various AI methodologies. However, by leveraging the experience of RIKEN R-CCS with COVID-19 simulations and quantitative risk assessment, there is an opportunity for a fruitful collaboration on risk assessment of infectious aerosol particles, utilising the nasal cavity geometry of the previous two tasks. This would provide a more personalised view on the problem of infection risk reduction, building on the previous award-winning research carried out by the Complex Phenomena Unified Simulation Research Team during the COVID-19 pandemic[2]. Corresponding activities are foreseen in the second period for Task 5.6.

While there are two capable simulation codes - m-AIA and CUBE, employed by the SDL FSE and the Complex Phenomena Unified Simulation Research Team, respectively, the results reported in this periodic report are achieved by using m-AIA. The primary reason is that, in contrast to CUBE, m-AIA is an open-source code, and it is easier to disseminate the research results and associated methodologies to a wider community. Nevertheless, the CUBE code has been optimised over the past decades for optimal performance on a series of supercomputers at R-CCS. The second phase of the project will therefore also look at CUBE and benchmark its performance on European systems as far as licences permit.

More details about m-AIA's computing performance can be found in Section 2. Subsequently, Section 3 presents the highlighted scientific results achieved in the first reporting period. It should be noted that this section only includes the results directly related to the HANAMI project, while further associated publications are presented in Section 9. As the exchange and collaboration with the Japanese partner is key to the success of this project, Section 4 expands on the details of collaborative activities. Next, a brief summary of work already achieved and the plan for the next phase of the project are described in Section 5. Computational resources that have been acquired within the reporting period to work on the tasks are presented in Section 6. Finally, Section 7 provides a summary and Section 8 provides brief conclusions, and Section 9 lists the full list of publications.

[2] Gordon Bell Special Prize for HPC-Based COVID-19 Research Awarded to Japanese Team for Novel Aerosolized Droplet Simulation https://www.acm.org/media-center/2021/november/gordon-bell-special-prize-covid-research-2021

2. m-AIA performance on HPC systems

The multi-physics simulation framework m-AIA has been extensively tested on several JSC supercomputers[3]. Tables 1-4 show the scaling test results across different systems, while Figures 1 and 2 display the scaling for Central Processing Unit (CPU) and Graphics Processing Unit (GPU)-ported variants of the code, respectively.

Table 1 m-AIA performance on Hazel Hen, JURECA-DC and CLAIX supercomputers.

CFD Method	Number of cells (millions)	HPC system	number of cores / runtime [s]					
			384	758	1,536	3,072	6,144	12,288
Lattice-Boltzmann	1070	HAZEL HEN	110.49	58.70	30.65	16.41	8.96	4.97
		JURECA-DC	156.28	87.43	46.21	21.52	-	-
Thermal Lattice-Boltzmann	1070	JURECA-DC	334.14	183.09	95.95	47.84	-	-
		CLAIX	233.20	120.69	63.22	32.56	17.56	-

Table 2 m-AIA performance on the JUQUEEN supercomputer.

CFD Method	no. cells (M)	HPC system	number of cores / runtime [s]								
			1,024	2,048	4,096	8,192	16,384	32,768	65,536	131,072	262,144
Lattice-Boltzmann	1230	JUQUEEN	633.85	332.76	169.87	88.79	47.29	25.25	12.60	7.26	6.19

Table 3 m-AIA performance on the JUWELS Booster supercomputer.

CFD method	no. cells (million)	HPC system	number of threads / runtime [s]					
			256	512	1,024	2,048	4,096	8,192
Lattice-Boltzmann	158	JUWELS Booster	117.03	44.66	20.83	12.20	7.75	5.62
	1230		-	-	-	120.94	48.06	22.42

Table 4 m-AIA performance on the JUWELS Cluster supercomputer.

CFD method	no. cells (M)	HPC system	number of nodes (4 GPUs per node) / runtime [s]								
			1	2	4	8	16	32	64	128	256
Lattice-Boltzmann	134	JUWELS Cluster	135.61	71.54	45.93	27.82	16.38	11.06	-	-	-
	2097		-	-	-	-	307.76	174.24	93.27	58.79	38.01

The newest addition to JSC's supercomputers, JUPITER, underwent some initial scaling tests. More specifically, a small scaling test was carried out on JEDI, the first module of JUPITER. More thorough and large-scale testing will be carried out when JUPITER is officially opened and the performance is stabilized.

[3] JSC Supercomputers https://www.fz-juelich.de/en/ias/jsc/systems/supercomputers

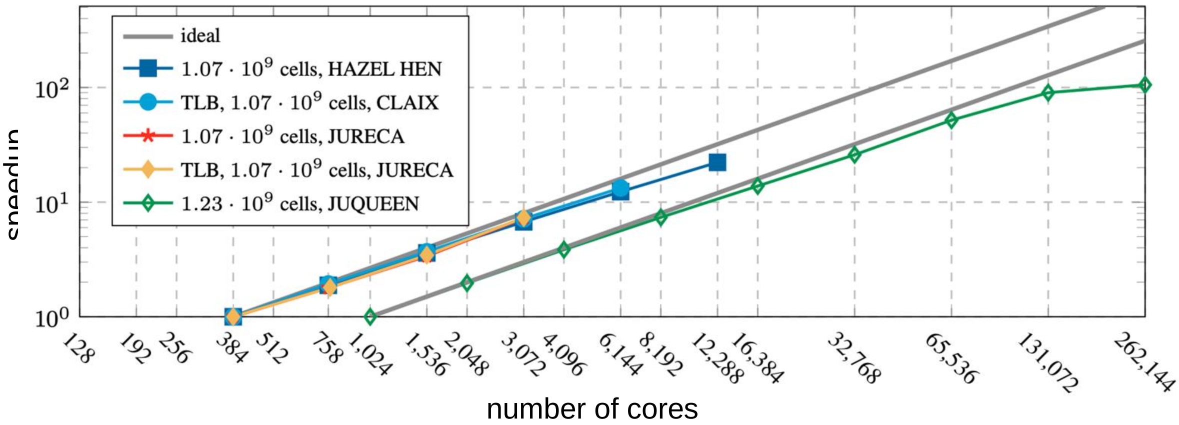

Figure 1: m-AIA scaling on CPU-based JSC systems for the (Thermal) Lattice-Boltzmann method.

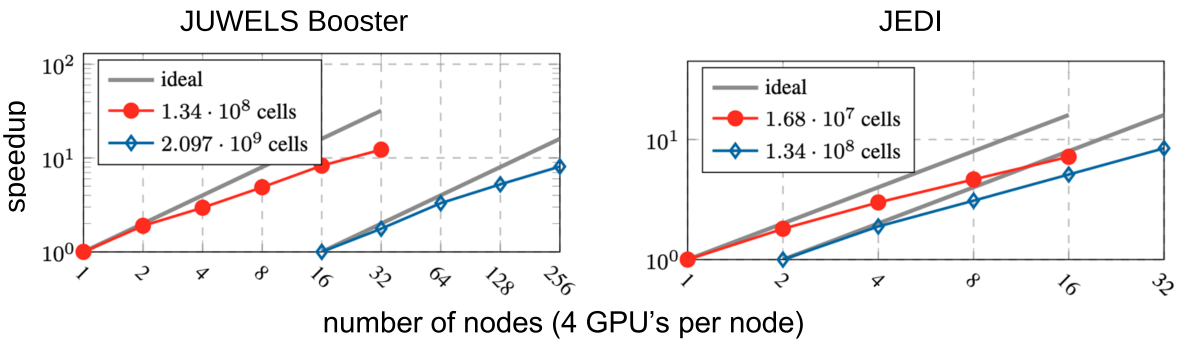

Figure 2: m-AIA scaling on GPU-based JSC systems for the Lattice-Boltzmann method.

Just recently, m-AIA has also been successfully ported to Fugaku, a flagship Japanese HPC system. No extensive scaling test has been done yet due to limited computational budget on the system, but this will be done in the foreseeable future.

3. Key scientific results achieved in the first reporting period

In the first reporting period, several ongoing research efforts led to the following publications, which fully align with the aforementioned Tasks 5.5 and 5.6 of HANAMI:

[P1] Patient-specific lattice-Boltzmann simulations with inflow conditions from magnetic resonance velocimetry measurements for analyzing cerebral aneurysms -
M. Rüttgers et al. (doi:10.1016/j.compbiomed.2025.109794)

This publication demonstrates the use of the m-AIA code to perform patient-specific CFD simulations of cerebral aneurysm hemodynamics by incorporating realistic inflow conditions obtained from magnetic resonance velocimetry. The methodology shows how MRI-derived velocity data can be directly coupled with high-fidelity Lattice Boltzmann simulations to capture complex, patient-specific flow fields in medical contexts.

While this study focuses on cerebral aneurysms, it represents an important extension of personalised CFD analysis from respiratory flows to complex vascular flows. By demonstrating patient-specific modelling of blood flow dynamics with realistic inflow data, it lays the foundation for developing AI-assisted surgery planning tools for aneurysm treatment, aligning directly with HANAMI's objective of advancing personalised medicine through high-fidelity, AI-enhanced simulations.

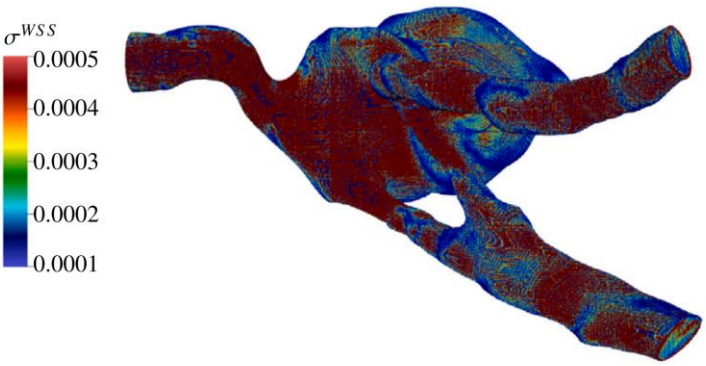

Figure 3: Wall shear stress inside the nasal cavity for a Lattice Boltzmann model based on the Carreau–Yasuda equation.

[P2] Towards a widespread usage of computational fluid dynamics simulations for automated virtual nasal surgery planning -
M. Rüttgers et al. (doi:10.1016/j.future.2025.107935)

This paper introduces a computationally efficient framework for CFD-based virtual planning of nasal cavity surgeries, such as septoplasty and turbinectomy. A hybrid method combining the lattice-Boltzmann approach with level-set-based interpolation allows simulation of surgical variations through a discrete set of geometry steps at single surgery interventions. This reduces the number of required simulations to as few as 21 per intervention. Previous methods rely on more costly coupling strategies, such as reinforcement learning or thermal modelling, which may still be appropriate for complex planning scenarios involving multiple intervention sites or thermal flow analysis. Despite this simplification, the method retains key predictive capabilities, optimising pressure loss and flow balance while reducing unnecessary tissue removal. Case studies demonstrate tissue savings of 12–25% and the use of a regression model to further reduce computational cost by 50%, with less than 4% prediction error.

This work supports HANAMI WP5 by delivering a clinically viable, automated CFD framework tailored for personalised medicine at the macroscopic level. By enabling efficient prediction of nasal airflow outcomes from surgical interventions, the study demonstrates how CFD can be integrated into routine clinical workflows. The hybrid method lays foundational work toward AI-assisted, patient-specific surgery planning tools envisioned in HANAMI.

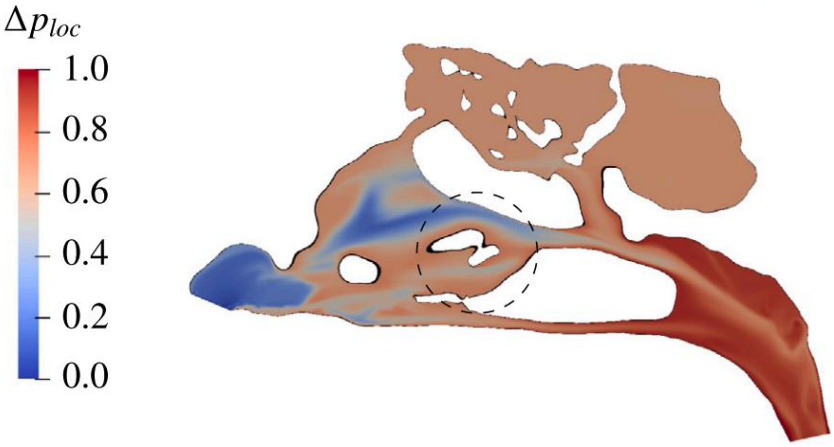

Figure 4: Normalised pressure loss after geometry modification between the inlets (nostrils) and the outlet (pharynx).

[P3] HydroGym-GPU: From 2D to 3D Benchmark Environments for Reinforcement Learning in Fluid Flows -
C. Lagemann, M. Rüttgers, et al. (doi:10.34734/FZJ-2025-02455)

This work introduces HydroGym-GPU, a GPU-accelerated extension of the HydroGym platform that integrates the highly parallelised lattice-Boltzmann solver of the m-AIA framework with RL workflows for fluid flow control. By enabling large-scale, three-dimensional CFD environments on modern GPU architectures, the platform removes a major barrier to studying realistic flow control problems. It provides standardised, open benchmark environments that support advanced RL algorithms in scenarios of significantly increased physical and computational complexity, addressing a critical gap between 2D academic examples and real-world 3D control challenges.

This development supports HANAMI WP5's vision of advancing AI-assisted, patient-specific simulations by laying the groundwork for integrating RL-based surgical planning tools into a robust, open-source framework. The close collaboration with Steven Brunton's group from the University of Washington ensures the application of state-of-the-art RL methodologies to large-scale biomedical CFD problems. Notably, the RL-based nasal surgery planning tools developed in HANAMI are intended to become part of this open platform, ensuring their long-term impact and accessibility for future clinical and research use.

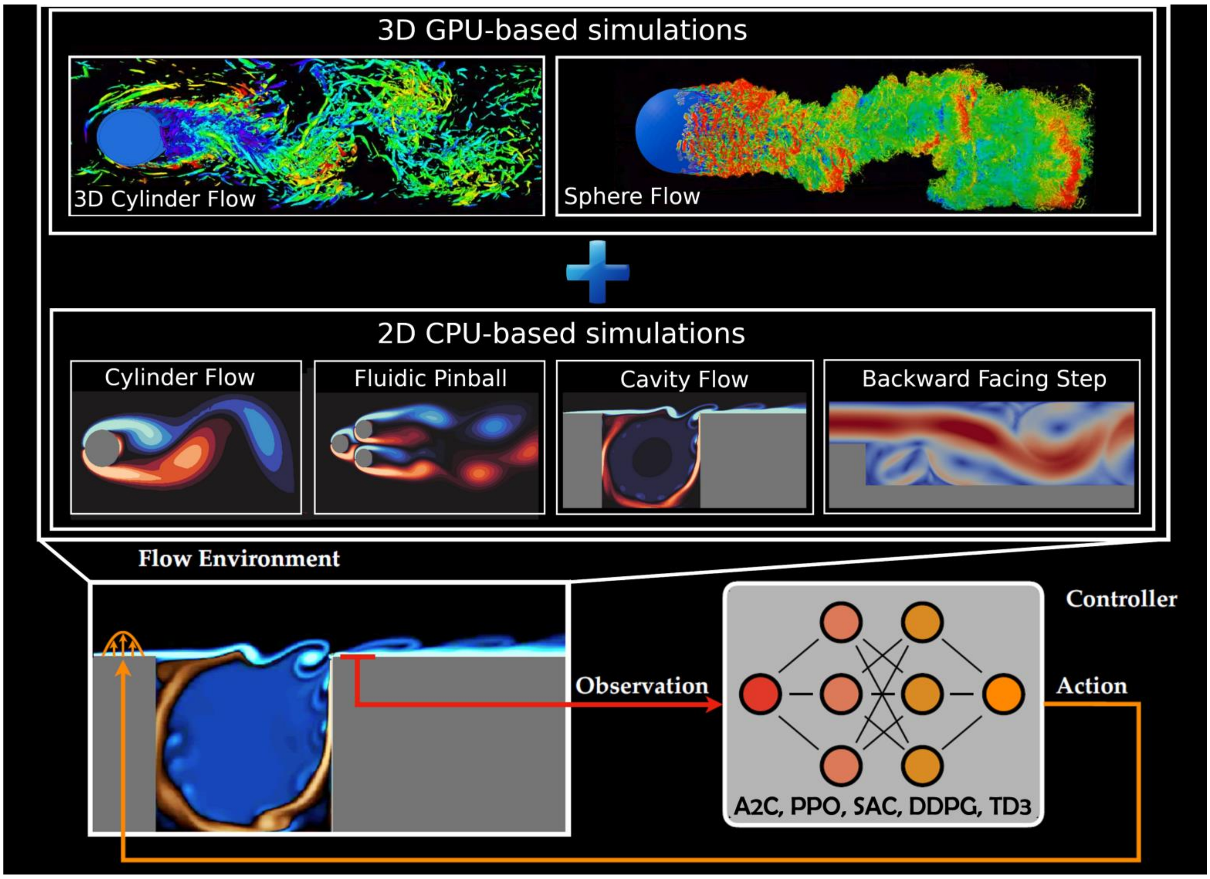

Figure 5: Flow configurations and benchmark algorithms included in the initial and extended HydroGym-GPU platform

[P4] Wet-Surface Modeling in Lattice-Boltzmann Simulations for Evaluating Surgery Impacts on the Humidity Transfer in Nasal Flows -
S. Ito, M. Rüttgers et al. (DOI: 10.34734/FZJ-2025-02479)

This study presents the first lattice-Boltzmann simulations using the m-AIA framework to explicitly model humidity fields in patient-specific nasal airflow, providing a more physiologically meaningful measure of the nose's conditioning ability than temperature alone. A novel wet-surface boundary treatment was implemented to account for latent heat effects from mucosal evaporation, dynamically influencing wall temperature and water vapour concentration. The study compares pre- and post-surgical (turbinectomy) nasal cavities, revealing that surgery reduces inspiratory pressure loss but leads to drier air reaching the back of the throat, matching the patient's reported symptoms.

This development represents an important step for HANAMI WP5. By moving beyond temperature-based conditioning metrics to predict full humidity fields, the approach offers a more accurate and relevant assessment of nasal surgery impacts on airflow and patient comfort. The validated wet-surface modelling approach will be integrated into the AI-assisted nasal surgery planning tool being developed in HANAMI, improving its ability to recommend surgical interventions that balance airflow efficiency with humidification performance.

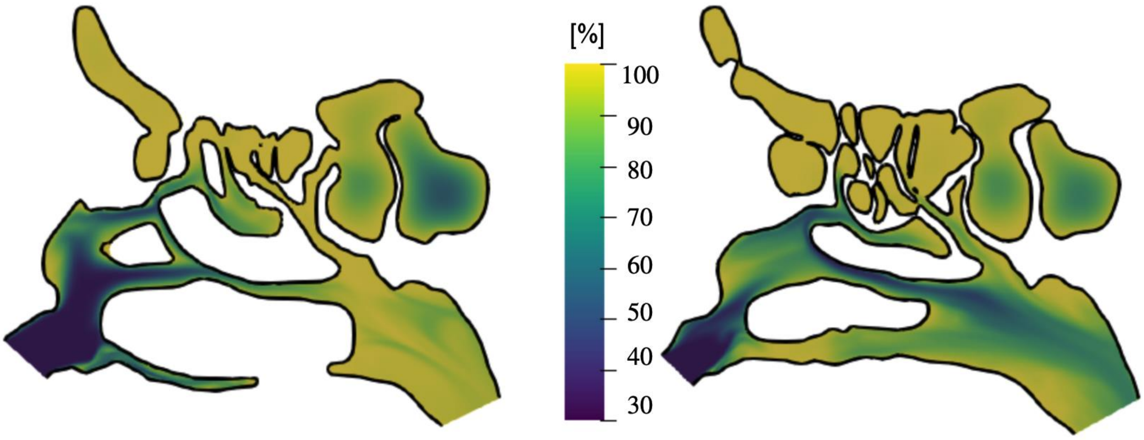

Figure 6: Humidity distribution for a cross-sectional area through the left nasal passage (from the patient's view) of the pre-surgical (left) and the post-surgical (right) cases.

[P5] Parallel Reinforcement Learning and Gaussian Process Regression for Improved Physics-Based Nasal Surgery Planning -
M. Rüttgers et al. (doi:10.1007/978-3-031-85703-4_6)

This paper presents a novel approach for physics-based virtual nasal surgery planning that combines parallel RL with Gaussian process regression (GPR) to optimise surgical outcomes efficiently. By leveraging parallel RL agents to explore surgical parameter spaces and training GPR surrogate models for rapid prediction of fluid-dynamic outcomes, the method significantly reduces the number of expensive CFD simulations required for surgery planning. Demonstrated on patient-specific nasal geometries, this approach delivers high-quality surgical recommendations with reduced computational cost, making AI-driven CFD planning more practical for clinical use. The work was recognised with the **Best Paper Award** at the PPAM conference in Ostrava, September 2024.

The integration of GPR into the workflow benefited substantially from the expertise of the Japanese project partners, enabling efficient surrogate modelling of CFD results. This close collaboration showcases the value of combining domain knowledge, HPC resources, and AI methodologies across institutions to deliver practical, clinically relevant tools for personalised medicine.

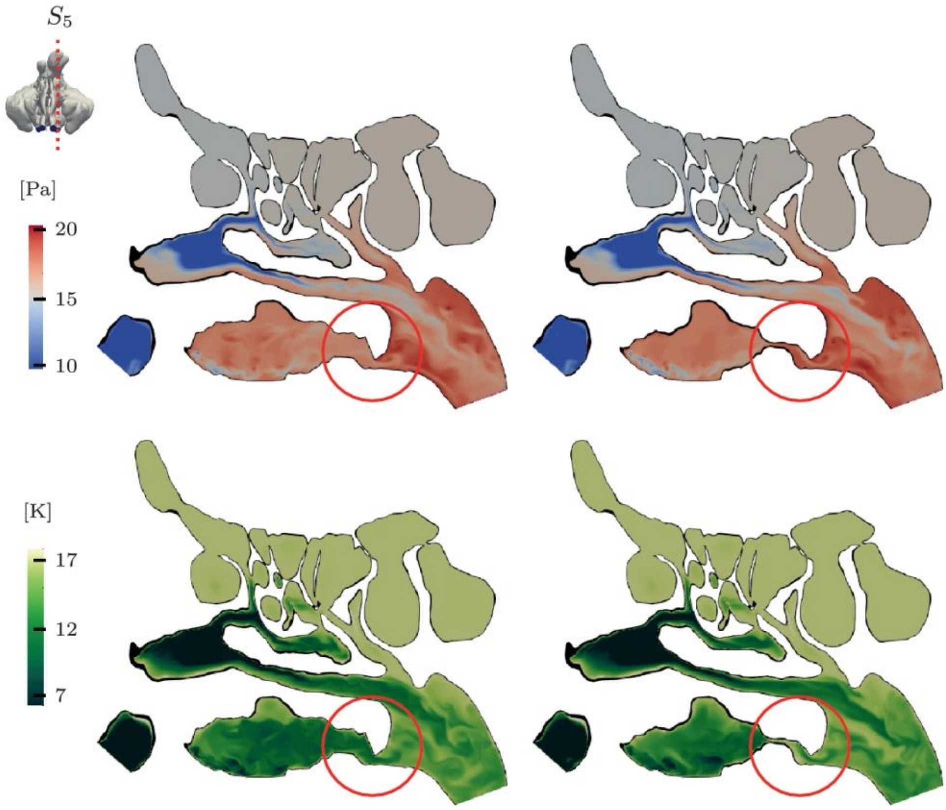

Figure 7: Total pressure loss [top] and temperature increase [bottom] between the inlets and locations inside of the nasal cavity for (αC,αD)=(0.85, 0.25) [left] and (αC,αD)=(0.6, 0.15) [right] at the cross-sectional area $S5$, which is illustrated by the dashed line in this figure. The red circles highlight the region of large deviations between the two cases.

4. Knowledge and software exchange between Forschungszentrum Juelich and R-CCS

Monthly meetings take place to update on the progress of the Joint Laboratory for Extreme Scale Computing (JLESC) Project "Deep Neural Networks for CFD Simulations". The groups exchange primarily on the topics of PINNs and Graph Neural Networks (GNNs). This collaboration has been fruitful, with both groups contributing to one joint publication in a JLESC special issue [P6] and another manuscript currently under review. For PINNs, the research contributed to benchmarking the performance of PINNs to traditional Deep Neural Networks (DNNs) for classical flow problems when data is sparse and localised. Also, the generalizability of Physics-Informed Deep Operator Network (PI-DeepONet) is investigated in the joint work. For GNNs, the groups are looking into the accuracy and performance of physics-aware and data-free GNNs for problems in urban flows and combustion. This work is expected to contribute to a better understanding of the effect of integration of physical laws in training Neural Networks (NNs) for CFD applications.

In addition, the SDL FSE team member Alex Krochak visited R-CCS in June 2025 to compile, set up, and test the multi-physics simulation code m-AIA from RWTH Aachen on Fugaku. As Fugaku features a different chip architecture for its login and compute nodes, cross-compilation proved to be difficult. Nonetheless, the code was eventually successfully compiled with the use of the Fujitsu C++ compiler together with the Clang compilation flag option to allow for the C++17 standard that is used by m-AIA (the standard Fujitsu compiler unfortunately does not offer full C++17 support). A merge request to include the full configuration steps necessary for Fugaku compilation is currently in progress as m-AIA is transitioning to C++20 standard support. It is planned to retry the compilation with C++20 standard libraries and update the merge request accordingly in the next few months.

In addition to the m-AIA compilation, part of the research stay at R-CCS was specifically dedicated to the knowledge exchange with Complex Phenomena Unified Simulation Research Team members. It is planned to include Dr. Rahul Bale, one of RIKEN's experts on CFD simulation for quantitative infection risk assessment, as a collaborator for future HANAMI-related personalised medicine work at JSC, as part of Task 5.6. Additionally, Krochak gave a presentation to the members of the R-CCS team and M.Sc. students under Prof. Tsubokura's supervision at Kobe University. The topic of the presentation was the use of AI methods for large-eddy simulation closure modelling in CFD.

5. Future work in the second HANAMI period

Initial efforts by Juelich in the first reporting period were directed towards setting up the required tools necessary for the successful integration of AI methodologies into m-AIA CFD workflows. Juelich has successfully achieved the main goals of this task. The publications presented in Section 2 [P1, P2, P3, P4] underline the improvements in physical modelling and in enabling AI components, such as RL, to improve simulation performance via accurate AI-augmentation. This foundation allowed for ultimate additions of various AI components to the CFD pipeline for nasal cavity simulations, as it is described in the first part of Task 5.6, see for more detail [P5].

Thus, the remainder of the project will focus on the second part of Task 5.6, namely, providing a quantitative CFD-based infection risk assessment, as well as improving the structure and ease-of-use of previously developed tools. To this end, a software repository has been hosted on the AI4HPC open-source library of models[4]. This repository is currently being developed to allow these tools to be accessed and used by anyone interested.

For the infection-risk assessment, a combined geometry of both the internal nasal cavity and the external surroundings is used to compute the trajectory of viral droplets and their likelihood of entering the nasal cavity, see Figure 8 for reference. The initial conditions of these droplets, i.e., their initial position, velocity, diameter, and density, are varied to study the effect of these parameters on the likelihood of particle deposition and thus on an infection. Using the initial particle condition, such as its position and velocity, together with its ultimate probability of deposition, can be used to enhance already existing simulations which used simpler deposition models, as well as to provide physical insights on how to reduce infection risks by accounting for such effects. For example, some simulations assume that the particle will be deposited inside the airway as soon as it's within a certain distance of a nasal opening, and do not account for particle velocity. The reader is referred to the next section, particularly to the 2025 compute time subproject, for more details of the work planned.

[4]AI4HPC Nasal Cavity repository https://gitlab.jsc.fz-juelich.de/CoE-RAISE/FZJ/ai4hpc/ai4hpc-dev/-/tree/nasal-cavity?ref_type=heads

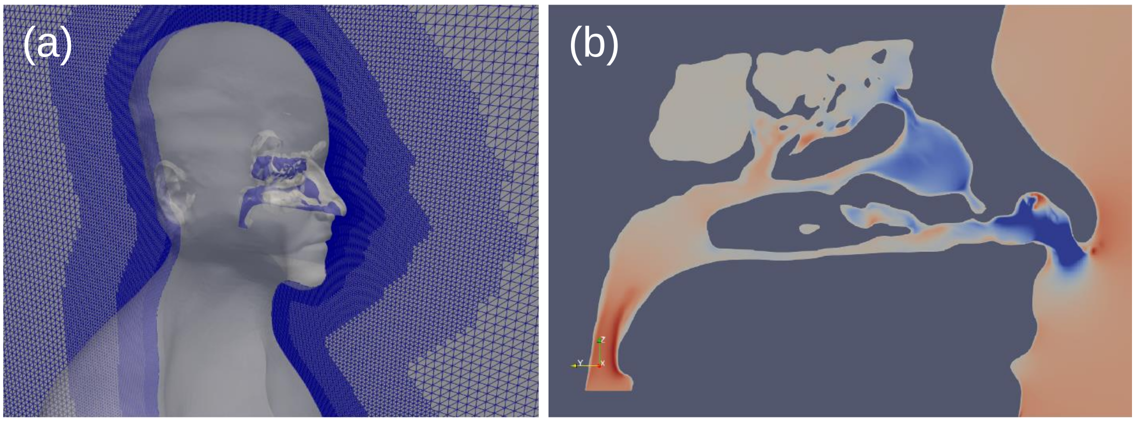

Figure 8 - Combination of external and internal geometries for future HANAMI simulations (a). Velocity magnitude through a slice of nasal cavity internal geometry, preliminary simulation (b).

6. Computational resources

The activities described in Section 2 and Section 3, as well as those foreseen in the future, see Section 5, can only be performed with sufficient HPC compute time. Much of the development involved training of AI models and, hence, for better efficiency, required the usage of GPUs. Therefore, compute time proposals were filed containing requests for performing simulations on CPU-based systems, and for performing training on GPU partitions.

Specifically, two VSR compute time proposals at JSC were successful in 2024 and 2025, each with a runtime of one year[5]. They received compute time grants amounting to the budgets listed in Table 5 below. The corresponding proposals were jointly prepared between JSC and R-CCS. The main Principal Investigator (PI) is the leader of the SDL FSE, Dr. Andreas Lintermann. As co-PI, Dr. Junya Onishi from R-CCS contributed to the proposal and to the implementation of the work together with the team members from the SDL FSE.

While the 2024 compute time project mainly concentrated on the activities in Task 5.5, the 2025 compute time project (05.2025 - 04.2026) also contains a sub-project targeted at the infection-risk analysis for trans-nasal-cavity flow as planned in Task 5.6. Specifically, the following tasks are part of the compute time project:

- A combination of the internal and external flow domains to numerically simulate the process of inhalation of viral particles, i.e., droplets containing viral matter, in the form of Lagrangian particles transported by the flow.
- The particles are distributed with varying density, diameter, initial velocity, and initial position to provide a realistic setup for analysis.
- The simulations are performed with the lattice-Boltzmann fluid mechanics solver and the Lagrangian particle tracking modules of the multi-physics open-source simulation framework m-AIA.
- A successful implementation of these tasks will provide data-driven assessment on the probability of inhalation of viral particles by healthy patients in clinical environments, such as waiting rooms, or in public transportation, depending on the initial position of the particles.

For the VSR projects, the Jülich Research on Exascale Cluster Architectures (JURECA) DC system is used, which consists of multiple partitions, however, only the JURECA DC CPU and GPU partitions are of relevance for the implementation of Project 3. The JURECA DC module containing both the CPU and GPU partitions has (as of 07/2025) 480 standard compute nodes, each equipped with two AMD EPYC 7742 with 2 x 64 cores, clocked at 2.25 GHz. The 192 accelerator nodes are additionally equipped with four NVIDIA A100 GPUs, each with 40 GB HBM2e. The interconnect is a Mellanox InfiniBand HDR (HDR100/HDR) DragonFly+ network[6].

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[5] VSR Compute Time call https://www.fz-juelich.de/en/ias/jsc/systems/supercomputers/apply-for-computing-time/vsr

[6] JURECA confiugration https://apps.fz-juelich.de/jsc/hps/jureca/configuration.html

For the activities that have taken place during the research visit described in Section 4.3 and beyond, the compute time allocation on Fugaku of the Complex Phenomena Unified Simulation Research Team at R-CCS is used. The Fugaku system has 158,976 nodes, each node containing 48 Armv8.2-A SVE 512-bit cores and additional assistant cores, as well as 32 GB HBM2 memory. The network topology is a Tofu Interconnect D[7].

Table 5: Compute time grants received during the first reporting period.

System	Budget	Timeline	Access
Improved Diagnostics of Respiratory Flows Using a Lattice-Boltzmann Method and Machine Learning Techniques			
JURECA DC CPU	1.76 M. core-h	from 05.2024 to 04.2025	SDL FSE and Dr. Junya Onishi
JURECA DC GPU	2.60 M. core-h	from 05.2024 to 04.2025	SDL FSE and Dr. Junya Onishi
Improved Diagnostics of Respiratory Flows Using a Lattice-Boltzmann Method and Machine Learning Techniques - extension proposal			
JURECA DC CPU	1.22 M. core-h	from 05.2025 to 04.2026	SDL FSE and Dr. Junya Onishi
JURECA DC GPU	1.57 M. core-h	from 05.2025 to 04.2026	SDL FSE and Dr. Junya Onishi
Establishment of a unified method for solving complex and composite phenomena and innovative manufacturing through data science integration			
Fugaku	5 M. node-h	from 04.2025 to 03.2026	RIKEN Complex team and Alex Krochak

[7] Fugaku configuration https://www.fujitsu.com/global/about/innovation/fugaku/specifications/

7. Summary

In the first period of HANAMI, Project 3 has made strong progress in using and improving CFD workflows for personalised medicine with AI components, as well as improving the overall physical modelling and computation performance. New AI methods, such as super-resolution imaging, PINNs, RL, and wet-surface modelling, were integrated into the simulation pipeline, improving the physical accuracy and reducing the overall simulation effort. This improved the technology readiness level of CFD workflows for personalised medicine.

The open-source m-AIA code performed well across several JSC supercomputers in Germany and was successfully ported to Fugaku in Japan. An evaluation of the code performance on Fugaku's Fujitsu A64FX ARM processors is planned soon.

Close collaboration with R-CCS, especially with the Complex Phenomena Unified Simulation Research Team, played a key role. Outcomes included software integration, regular knowledge exchange, and collaboration towards an infection-risk model based on Lagrangian particle tracking simulation(s) in combined internal/external geometries.

The next steps include refining the simulation tools via the AI4HPC platform and working towards the infection-risk model.

Overall, the main goals of the project have already been achieved and documented through various peer-reviewed publications, and this project successfully demonstrates how the combination of CFD and data-driven methods can enhance patient-specific treatment.

8. Conclusions

This mid-term deliverable highlights the coordinated progress achieved across the three WP5 projects, reflecting the strong collaborative efforts between European and Japanese partners. The work completed demonstrates HANAMI's capacity to co-develop advanced computational tools and methodologies that operate across molecular, cellular, and organ-level biological modelling in the life sciences domain.

These collaborations have laid the groundwork in Project 1 for exascale-capable molecular dynamics simulations, through the integration of a scalable Fast Multipole Method (FMM) into GROMACS, enabling efficient long-range electrostatics computations at the scale of entire cells. In Project 2, joint activities with Japanese partners have enabled the full integration of Large Language Models (LLMs) for network reconstruction and pathway modelling that will be essential for scaling multi-scale cellular simulations. Project 3 has advanced AI-assisted CFD workflows for personalised medicine by integrating methods like super-resolution imaging, PINNs, reinforcement learning, and wet-surface modelling. These enhancements improved physical accuracy while reducing the computational cost of simulation. The open-source m-AIA code showed strong performance on JSC systems and was successfully ported to Fugaku. A simulation for risk quantification of viral infection through inhalation is currently in progress.

Together, these achievements provide a strong technical and collaborative foundation for the second half of the project, which will focus on further scaling, deeper integration across projects, and the continued strengthening of European-Japanese collaboration to advance personalised medicine through exascale-ready biomedical modelling tools.

9. Full list of publications

The following lists the key peer-reviewed articles that have been published during the first reporting period in renowned journals (papers [P1, P2]). The paper [P5] won the Diploma Best Paper Award (winner for workshops) at the Parallel Processing and Applied Mathematics (PPAM 2024) Conference, which took place in Ostrava, Czech Republic, September 8 - 11, 2024.

[P1] Rüttgers, M., Waldmann, M., Ito, S., Wüstenhagen, C., Grundmann, S., Brede, M., & Lintermann, A. (2025). Patient-specific lattice-Boltzmann simulations with inflow conditions from magnetic resonance velocimetry measurements for analyzing cerebral aneurysms. *Computers in Biology and Medicine*, Vol. *187*, 109794. https://doi.org/10.1016/j.compbiomed.2025.109794

[P2] Rüttgers, M., Waldmann, M., Hübenthal, F., Vogt, K., Tsubokura, M., Lee, S., & Lintermann, A. (2026). Towards a widespread usage of computational fluid dynamics simulations for automated virtual nasal surgery planning. *Future Generation Computer Systems*, Vol. *174*, 107935. https://doi.org/10.1016/j.future.2025.107935

[P3] Lagemann, C., Rüttgers, M., Gondrum, M., Meinke, M., Schröder, W., Lintermann, A., & Brunton, S. L. (2025). HydroGym-GPU: From 2D to 3D Benchmark Environments for Reinforcement Learning in Fluid Flows. *Forschungszentrum Jülich Technical Report*. https://doi.org/10.34734/FZJ-2025-02455

[P4] Ito, S., Rüttgers, M., Waldmann, M., & Lintermann, A.(2025). Wet-Surface Modeling in Lattice-Boltzmann Simulations for Evaluating Surgery Impacts on the Humidity Transfer in Nasal Flows. *Forschungszentrum Jülich Technical Report*. https://doi.org/10.34734/FZJ-2025-02479

[P5] Rüttgers, M., Hübenthal, F., Tsubokura, M., & Lintermann, A. (2025). Parallel Reinforcement Learning and Gaussian Process Regression for Improved Physics-Based Nasal Surgery Planning. In R. Wyrzykowski, J. Dongarra, E. Deelman, & K. Karczewski (Eds.), *Parallel Processing and Applied Mathematics (PPAM 2024). Lecture Notes in Computer Science (LNCS)* Vol. 15581, pp. 79–96. Springer. https://doi.org/10.1007/978-3-031-85703-4_6

[P6] Puri, R., Onishi, J., Rüttgers, M., Sarma, R., Tsubokura, M., & Lintermann, A. (2024). On the choice of physical constraints in artificial neural networks for predicting flow fields. *Future Generation Computer Systems, Vol. 161*, pp. 361–375. North-Holland. https://doi.org/10.1016/j.future.2024.07.009

[P7] Liu, X., Rüttgers, M., Quercia, A., Egele, R., Pfaehler, E., Shende, R., Aach, M., Schröder, W., Balaprakash, P., & Lintermann, A. (2024). Refining computer tomography data with super-resolution networks to increase the accuracy of respiratory flow simulations. *Future Generation Computer Systems, Vol. 159*, pp. 474–488. North-Holland. https://doi.org/10.1016/j.future.2024.05.020

[P8] Rüttgers, M., Waldmann, M., Vogt, K., Ilgner, J., Schröder, W., & Lintermann, A. (2024). Automated surgery planning for an obstructed nose by combining computational fluid dynamics with reinforcement learning. *Computers in Biology and Medicine, Vol. 173*, 108383. Pergamon. https://doi.org/10.1016/j.compbiomed.2024.108383