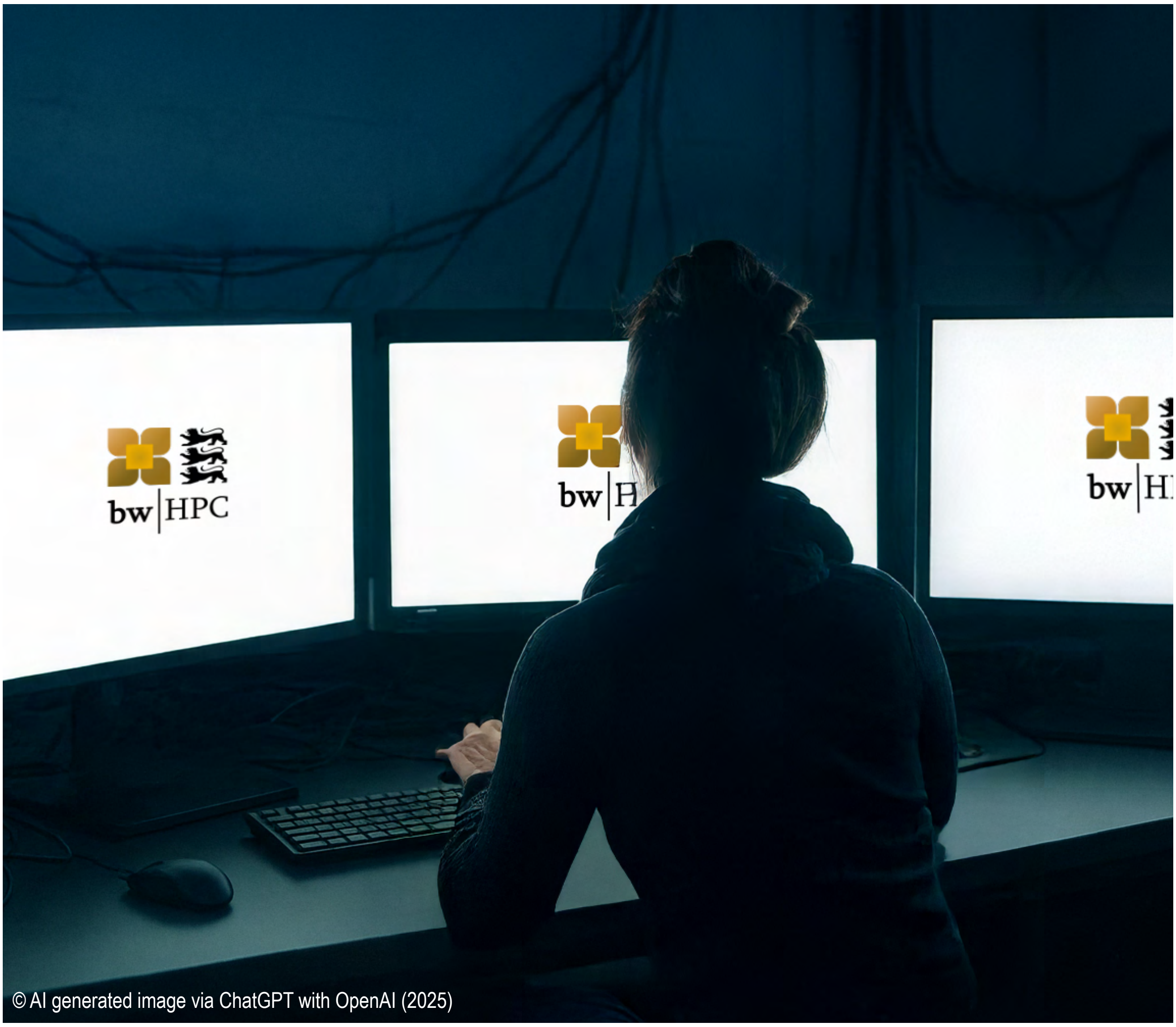
Newsletter

Edition No. 11, August 2025



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Commissioning NEMO2

Freiburgs new Supercomputer advances Neuroscience, Elementary Particle Physics, Microsystems Technology, and Materials Science

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The University of Freiburg officially put the new high-performance computer NEMO2 into operation today. It replaces the predecessor cluster NEMO, which has been in operation since 2016. The supercomputer is available for research projects by Baden-Württemberg scientists in the fields of neuroscience, elementary particle physics, microsystems technology and materials science.

As part of the tenth bwHPC Symposium, the bwForCluster NEMO2 was inaugurated by the Rector of the University of Freiburg, Prof. Dr Kerstin Krieglstein, and Ministerial Director Dr. Hans J. Reiter from the Baden-Württemberg Ministry of Science, Research and the Arts (MWK). Ministerial Director Reiter emphasised the importance of high-performance computers such as NEMO2 for science-driven innovation in Baden-Württemberg.

Compared to its predecessor, the new high-performance computer NEMO2 has twice as many computing cores, which corresponds to the computing power of around 5,000 standard laptops. This enables scientists to simulate more complex processes and analyse larger amounts of data. The supercomputer also contains special computing nodes for AI applications and research, which will be further expanded in 2025. Since the inauguration of NEMO in 2016, 643 researchers from 7 universities have used the high-performance computer and produced around 660 publications. NEMO2 was funded by the German Research Foundation (2.1 million euros), the state of Baden-Württemberg (1.5 million euros) and individual research groups (600,000 euros), totalling 4.2 million euros. The high-performance computer is part of the bwHPC network of supercomputers, which is available to students and researchers at Baden-Württemberg‘s universities.

Rector Kerstin Krieglstein emphasised the importance of NEMO2 for the further development of the digital research infrastructure at universities in Baden-Württemberg and as a hub for interdisciplinary research. Prof. Dr Stefan Rensing, Vice-Rector for Research and Innovation, underlined the new opportunities that NEMO2 opens up, particularly in the field of artificial intelligence.

Freiburg, 26 September 2024

Further informations:

- University of Freiburg
- Badische Zeitung (payable content)
- Ministerium für Wissenschaft, Forschung und Kunst Baden-Württemberg via LinkedIn
- NEMO 2 Wiki: Everything you might want to know about Registration, Login and Training Courses

New bwSupport Portal

Starting February 19, 2025, our long-running bwSupport Portal, hosted at KIT, will appear in a new look and feel. The new portal, based on the open-source platform Zammad, offers a more modern design, a faster interface, and additional features for improved high-level support. The new system is accessible at https://www.bwhpc.de/supportportal.

The federated login is available through bwIDM. Tickets can be created by clicking the „+“-symbol in the bottom left corner. A specific support unit can be selected using the search bar or navigating the arrows in the drop-down menu. A visual guide is available at the bwHPC Wiki.

Further informations:

- Zammad
- Support Portal
- Visual Guide
- https://www.scc.kit.edu/dienste/bwsupportportal.php

This article was mentioned in the kiz-Newsletter 06/25 of the University of Ulm.

Notice Regarding the Use of MathWorks Products in bwHPC

The use of MathWorks products at universities in the state of Baden-Württemberg is currently covered by a statewide academic license agreement, which took effect on April 1, 2023, and is valid until March 31, 2026.

Please take this defined timeframe into account when planning projects that rely on MathWorks software. Negotiations between the universities and MathWorks regarding a possible extension of the agreement beyond 2026 are currently ongoing. At present there is no confirmed outcome regarding a renewal.

For long-term research projects, we encourage considering alternative software solutions, including open-source options, where feasible.

User Survey 2025

Dear users of bwUniCluster and the bwForClusters,

to continuously improve our services, we conduct regular surveys to better understand your needs and adapt our offerings accordingly. Your feedback is essential: it not only helps us plan the procurement of new computing and storage resources, but also allows us to refine our support, training, and web presence.

The 2025 survey focused on various aspects of the bwHPC project — including resources, software, user support, training opportunities, and the online platforms we provide.

This year, we received 341 completed surveys (compared to 371 last year). We sincerely thank everyone who took the time to share their insights and suggestions. We are now carefully analyzing the results and will share the measures derived from your feedback in our next newsletter.

Thank you for your participation and support.

Warm regards,
Your bwHPC team

Success Stories

This article was mentioned in the kiz-Newsletter 06/25 of the University of Ulm.

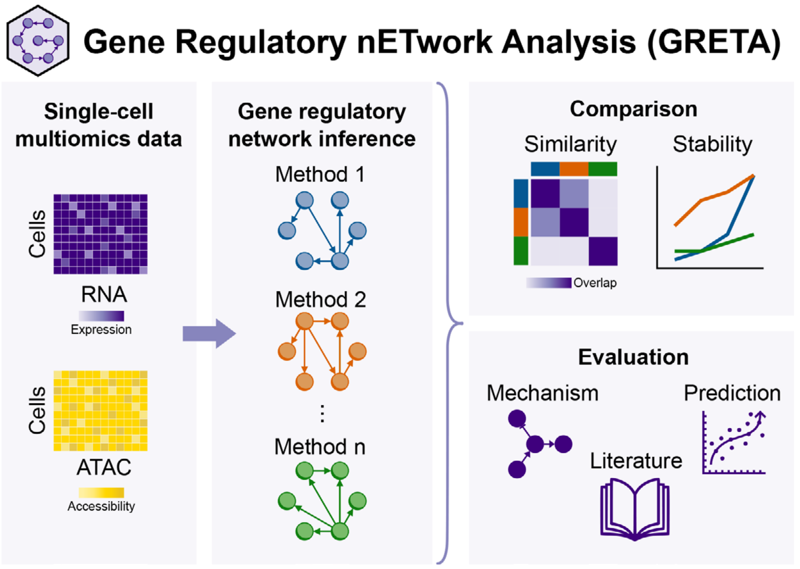
With approximately 1200 active users and over 500 publications annually, we are excited to introduce a new category to our website: The Success Stories. This section will showcase research highlights achieved using our bwHPC resources. We hope it will serve as an engaging resource for both newcomers and experienced users.

For newcomers, this section offers insights into the types of scientific calculations possible with HPC, and it may guide you to additional publications through references. For experienced users, it provides a platform to share your results with colleagues and the community. Additionally, featuring your work here enhances its visibility in search engine results. The Success Stories are driven by user contributions. If you wish to be featured, we encourage you to participate actively. Please complete the PDF form linked below and return it to us.

Further Information:

- https://www.bwhpc.de/success_stories.php
- https://www.bwhpc.de/downloads/bwHPC_Project_Report_Guideline_new.pdf

Comparison and Evaluation of Methods to infer Gene Regulatory Networks from Multimodal Single-Cell Data



Although all cells in the human body contain the same genetic information (DNA), they look and function differently. These differences are driven by gene regulation, where some genes control others in complex networks, making some genes be expressed in some cell types but not others. We can computationally generate these networks, known as gene regulatory networks (GRNs), using new technologies that measure individual cells. While many methods exist for making GRNs, it is unclear how well they actually work. In this study, we introduce a framework to evaluate and compare these methods.

To make our results reproducible, we implemented the latest GRN inference methods in a modular pipeline using Snakemake, a workflow management tool. Our framework leverages the Helix cluster to run jobs sequentially and SDS@hd for data storage. Using cluster resources was essential for this project, as GRN analysis demands significant computational power and storage space.

With our open-source framework, GRETA, we found that while these methods can recover regulatory interactions known from past research and make predictions from observational data, they struggle to predict causal relationships after perturbations. This highlights the need for further improvements. However, our framework now serves as a solid reference for measuring progress and comparing new methods.

Project Manager	Dr. Pau Badia i Mompel
Principal Investigator	Prof. Dr. Julio Saez Rodriguez
Affiliation	Heidelberg University, European Bioinformatics Institute (EMBL-EBI)
Project duration	3/2021 - Ongoing
Platform used	bwForCluster Helix, SDS@hd
bwHPC Domain	Medical Sciences
DOI of Publication	10.1101/2024.12.20.629764

Understanding Molecular Switches in Bacterial Gene Regulation

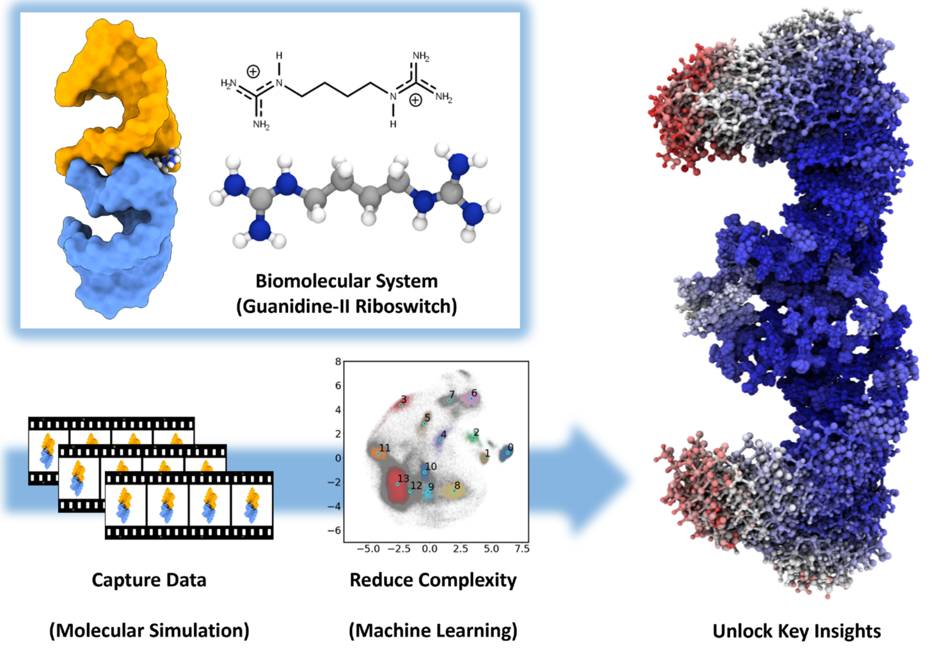


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Illustration of the guanidine-II riboswitch, a bivalent ligand and the computational workflow followed in this work.

Riboswitches are RNA-based regulatory elements that are improtant in bacterial gene expression. They act by changing their structure in response to small molecules called ligands. These dynamic structural changes, known as ‚switching', enable the riboswitch to modulate the expression of genes, highlighting its critical role in cellular regulation.

This study combines experimental investigations with extensive molecular dynamics simulations and machine learning techniques to explore the intricacies of the guanidine-II riboswitch. It is part of a family of riboswitches that sense guanidine, potentially enabling bacteria to utilize guanidine as a nitrogen source. A deeper understanding of their function and the underlying mechanisms not only provides valuable insights into fundamental microbial metabolism and gene regulation, but also offers promising applications in fields such as synthetic biology and pharmaceuticals, where controlling gene expression is key. By using specifically designed bivalent ligands, the study explored how these molecules bind to the riboswitch, impact the molecular interactions and trigger conformational changes of the RNA. Thus, they can play an important role for unravelling the detailed mechanisms of ligand-induced switching.

Simulating these structural transitions and binding events at the atomic scale poses significant computational challenges, requiring vast amounts of processing power. The bwHPC project provided the essential computational resources to manage these intensive simulations, and enabled the efficient analysis of large datasets through machine learning. This integration of computational power and data analysis was instrumental in discovering key aspects of ligand-riboswitch interactions.

In the molecular simulations, spontaneous ligand binding events were observed and a previously unknown, ligand-dependent base-stacking interaction in the guanidine-II riboswitch was identified. The results demonstrate that for this system, the bivalent ligands can significantly increase binding affinity compared to natural ligands. In vivo experiments confirmed these findings by highlighting cooperative binding effects.

This study paves the way for the development of high-affinity ligands that can modulate gene expression and highlights the importance of exploring ligand-dependent interactions in riboswitches. Future efforts will focus on further refining our understanding of the relationship between ligand binding and structural dynamics, potentially leading to new biotechnological tools and therapeutic strategies for controlling bacterial gene expression.

Project Manager	Dr. Jakob Steuer
Principal Investigator	Prof. Dr. Christine Peter
Affiliation	University of Konstanz
Project duration	bwHPC-S5 Phase II-III
Platform used	bwForCluster MLS&WISO, bwForCluster Helix
bwHPC Domain	Soft Matter
DOI of Publication	10.1093/nargab/lqae132

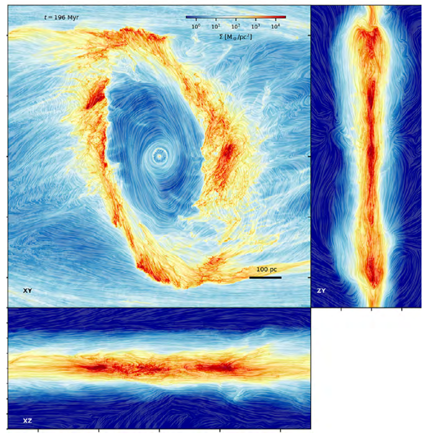
Magnetic Fields and Gas Dynamics in the Central Region of our Milky Way

The Milky Way has a prominent barred stellar structure in its central region. This significantly impacts the local gas flow, and torques exerted by this rigidly rotating structure drives copious gas inflow, with matter accumulating in a central structure called "The Central Molecular Zone" of about 100 pc in radius. The question of what causes the final sprint of the gas towards the central supermassive black hole is still largely unexplored as the torques from the bar are too small to explain the observed inflow in this very central region.

In this study we investigate the role that magnetic fields might play in this puzzle. Magnetic fields are ubiquitous in the Universe, and their dynamical evolution is intimately coupled to flow in the medium they permeate. As the interstellar medium drags magnetic field lines along on its way to build up the Central Molecular Zone, it can generate strong magnetic fields by compression. Turbulence then further enhances the magnetic fields through dynamo action, leading to values up to a thousand times higher than what we observe in our solar neighbourhood. This is a highly non-linear multi-scale process, and multi-phase magnetohydrodynamic (MHD) simulations are needed to address this problem. Specifically, we solve the time-dependent MHD equations in three dimensions using the moving-mesh code Arepo. The gas streams in an external potential that reproduces key features of the Milky Way, and the chemical state of the medium is followed by evaluating a complex chemical network in every cell at each time step. The code is efficiently parallelized and the simulations reported here had about 100 million cells.

We find that the magnetic field in the inner regions of the Milky Way can be decomposed into a regular time-averaged component and an irregular turbulent component. It aligns well with the velocity vectors of the gas in the Galactic plane and becomes increasingly poloidal at large heights. We also argue that the magneto-rotational instability (MRI) causes an inflow of matter towards the black hole in the center of the Galaxy. The gas velocity dispersion inferred from our simulations is lower than the measured values, suggesting that other processes such as stellar feedback are necessary to explain the observations. Dynamo action driven by differential rotation and the MRI amplifies the magnetic fields in the Galactic center region until they saturate at values of the order of 100 µG.

Project Manager	Prof. Dr. Ralf Klessen
Principal Investigator	Prof. Dr. Ralf Klessen
Author of this Article	Dr. Robin Tress
Affiliation	Heidelberg University, École Polytechnique Fédérale de Lausanne and 32 other institutions
Project duration	9/2016 - 11/2025
Platform used	bwForCluster BinAC & Helix, SDS@hd
bwHPC Domain	Astrophysics
DOI of Publication	10.1051/0004-6361/202450035



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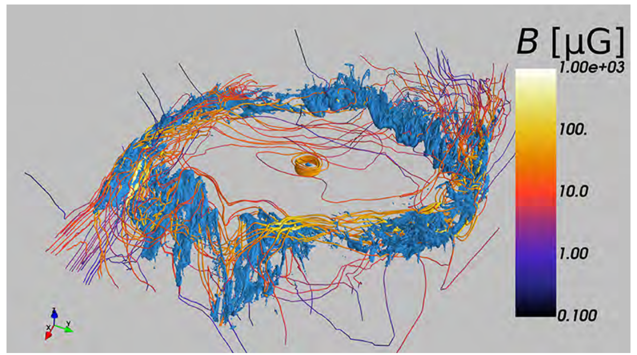
← Figure 8

Figure 10a →

Figure 10b →

Figure 8: Face-on and edge-on views of the interstellar medium in the central region of the simulated Milky Way analogue.The magnetic field lines are superimposed on the gas distribution. This structure is the so called "Central Molecular Zone" and it is fuelled by the gas streams seen coming in at the edges of the image, induced by the Galactic bar.

Figure 10 a and b: A 3D rendering of the simulated Central Molecular Zone. A few selected magnetic field lines are shown, coloured by their local intensity. These images help us understand the morphology of the magnetic field in the region, shaped by the complex gas motions.



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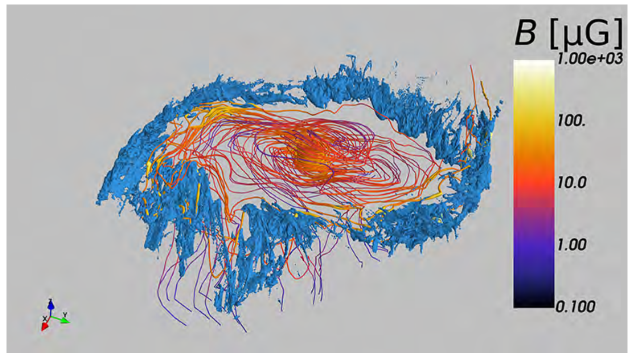

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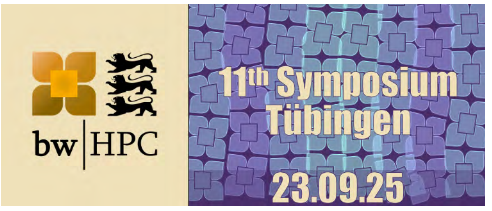
Upcoming Events



The event will take place on September 23, 2025, at Eberhard- Karls-Universität Tübingen. The symposium will feature a diverse program, including talks and poster sessions.
Registration is open. The registration deadline is September 5th, 2025.

Register here: https://uni-tuebingen.de/einrichtungen/zentrum-fuer-datenverarbeitung/dienstleistungen/server/computing/veranstaltungen/bwhpc-symposium-2025/registration/

Feel free to contact us at symposium2025@bwhpc.de

Upcoming Training Courses

- 01.09. - 10.10.25: Data Analysis with HPC, online @ HLRS Supercomputing Academy
- 08.09. - 12.09.25: Introduction to Computational Fluid Dynamics, on-site @ University of Stuttgart
- 23.09. - 26.09.25: Julia for High Performance Computing, on-site @ University of Stuttgart
- 13.10. - 17.10.25: Parallel Programming Workshop (MPI, OpenMP & advanced topics), on-site @ University of Stuttgart
- 20.10. - 10.11.25: Time Series Forecasting, online @ HLRS Supercomputing Academy
- 23.10. - 24.10.25: Scientific Visualization, on-site @ University of Stuttgart

For more courses visit: https://www.bwhpc.de/courses_a_tutorials.php

The next bwHPC-Newsletter will be published in winter 2025.
We wish you a nice summer!

Greetings from the bwHPC-Team

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