IAS Retreat 2025

Forschungszentrum Jülich

27 May 2025

Contents

IAS Retreat 2025

27 May 2025
Forschungszentrum Jülich, Central Library

Welcome

The IAS Retreat is intended to bring together IAS members and related institutes to meet, exchange ideas and get to know each other. You can look forward to a full day of plenary presentations of institute divisions, poster sessions with preceding spotlight talks, a session on large research projects and infrastructures relevant to the IAS, a Senior Investigators Meeting, a Scientific Support Meeting, and lots of breaks with food and drinks and time to chat.

The three most interesting, appealing or best presented posters will be awarded at the end of the event. Please vote for your favourite poster by 5 p.m. on 27 May via the QR code.

The **Junior Researchers Event** takes place in advance as a satellite event on 22 May 2025, 11:00-16:00 at the campus of the Forschungszentrum Jülich.

Thank you to all speakers and participants for being part of IAS Retreat 2025!

Organizing team

Sonja Grün (IAS-6) & Tom Luu (IAS-4)
Anne Elfgen (IAS-6) & Martina Reske (IAS-6)
Daria Abels (IAS-8), Carole Babelot (IAS-7), Younes Bouhadjar (PGI-15),
Vania Calandrini (INM-9), Zhuo Cao (IAS-8), Michael Denker (IAS-6),
Katharina Immel (IAS-9), Moritz Kern (IAS-6), Janine Lehm (IAS-6),
Saskia Meissner (IAS-6), Gregor Michalicek (PGI-1), Tobias Michels (IAS-6),
Petra O'Brien (IAS-6), Marisol Ripoll (IAS-2), Thorben Schoepe (PGI-15),
Erenus Yildiz (IAS-8), Robert Speck (JSC), Xuan Zhao (IAS-8)

Assistance

Anne Elfgen and Martina Reske can be contacted before, during and after the conference at:
scico-ias-6@fz-juelich.de
Anne: 02461-61-9468 or 0160-95640572
Martina: 02461-61-1916

Program

Online program: https://events.hifis.net/event/2100/page/629-program

Time	Sessions	Meetings
08:30-09:00	**Registration & Welcome Coffee** Foyer	
09:00-09:10	**Welcome Address** Lecture Hall, Chair: Sonja Grün Ulf G. Meißner, IAS Managing Director Laurens Kuipers, Member of the Board of Directors (VS-I)	
09:10-11:00	**Presentations of the Institute Divisions, Part I** Lecture Hall, Chair: Marisol Ripoll **IAS-2** ***Minimal Physical Modeling of Living Systems*** - Thorsten Auth, Jens Elgeti **IAS-4** ***Nuclear Lattice Effective Field Theory in a Nutshell*** - Fabian Hildenbrand ***Engineering Topological Phases in Quantum Nanosystems*** - Lin Wang **IAS-6** ***Introduction to IAS-6*** - Sonja Grün ***Physics of AI*** - Moritz Helias **IAS-7** ***Shaping the Future of Crowd Safety: From Flames to Footsteps*** - Lukas Arnold and Mohcine Chraibi **IAS-8** ***Retrieval of Sun-Induced Plant Fluorescence from Hyperspectral Imagery*** - Jim Buffat ***Galaxy Morphology Classification with Counterfactual Explanation*** - Zhuo Cao	
11:00-11:30	**Coffee Break & Group Photo** Foyer	
11:30-11:50	**Spotlight Talks, Part I** Lecture Hall, Chair: Abigail Morrison ***Exascale Computing for Skyrmion Simulations*** - Nihad Abuawwad (#1) ***Supercomputing in a Browser - Easy access to WebTools for Increased Productivity*** - Jens Henrik Goebbert, Tim Kreuzer (#43) ***Hadron Physics with the Jülich-Bonn Model: Determining the Light Baryon Resonance Spectrum*** - Oleh Luniachek, Deborah Ronchen, Christian Schneider (#65) ***Vortex Formation and Odd Viscosity in a Chiral Active Fluid*** - Joscha Mecke (#69) ***Combining Socio-Psychological Pedestrian Dynamics with AI and Simulation Tools*** - Ezel Üsten (#97)	**Scientific Support Meeting** (30-60 min) Room 338
11:50-12:40	**Poster Session, Part I (odd numbers)** Foyer	
12:40-13:40	**Lunch** Foyer	

13:40-15:30	**Presentations of the Institute Divisions, Part II** Lecture Hall, Chair: Erenus Yildiz **IAS-9** ***Materials Data Science and Informatics*** - Stefan Sandfeld **JSC** ***The Futures of Computing at JSC*** - Robert Speck **INM-9** ***Computational Biomedicine - Developing and Using Molecular Simulation, Machine Learning, and Bioinformatics Tools to Investigate Neurotransmission in the Human Brain*** - Giulia Rossetti **PGI-1** ***An IAS Perspective on the Peter Grünberg Institut 1 - Quantum Theory of Materials*** - Gregor Michalicek **PGI-15** ***Neuromorphic Principles for Self-Attention*** - Emre Neftci	
15:30-15:50	**Spotlight Talks, Part II** Lecture Hall, Chair: Vania Calandrini ***Leveraging LLMs and Ontologies for Simulation Data Extraction and Exploration*** - Elaheh Akhoundi (#2) ***Event-Driven Eligibility Propagation: Combining Efficiency with Biological Realism*** - Agnes Korcsak-Gorzo (#56) ***Cognitive Maps in Brains and Machines*** - Sven Krausse; Alpha Renner (#60) ***Summation Compression for Very Low-Rank Adaptation*** - Alessio Quercia (#84)	
15:50-16:40	**Poster Session, Part II (even numbers)** Foyer	
16:40-16:50	**Short Break** Foyer	
16:50-17:50	**Large Research Projects and Infrastructures** Lecture Hall, Chair: Robert Speck ***JUPITER - Pushing Technical and Scientific Boundaries to the Exascale Level*** - Benedikt von St. Vieth ***Better Software Better Research*** - Claire Wyatt ***Fostering Interdisciplinarity: The Jülich Neuromorphic Computing Alliance*** - Abigail Morrison ***Rhine-Ruhr Center for Scientific Data Literacy - An Introduction and Recent Activities*** - Katharina Immel ***Helmholtz AI Consulting - supporting AI innovation in Helmholtz*** – Stefan Kesselheim	
17:50-18:00	**Closing Remarks, Report from the Junior Investigators Event & Poster Prize** Lecture Hall Tom Luu, Sonja Grün, Katharina Immel	
18:15-19:15		**Senior Investigators Meeting** Foyer

Senior Investigators Meeting
A meeting of senior investigators (i.e. senior postdocs, team leaders, group leaders, directors, …) to get to know each other and exchange ideas and perspectives on, among others, cooperation within the IAS, leadership matters, and communication.

Scientific Support Meeting
An informal get-together of those IAS members supporting scientific activities at the IAS (i.e. secretaries, coordinators, IT staff, …).

Poster Contributions

P-001 – Exascale computing for skyrmion simulations

Nihad Abuawwad, Peter Grünberg Institute (PGI-1), Forschungszentrum Jülich

Authors: Nihad Abuawwad, Daniel Wortmann, Gregor Michalicek, Stefan Blügel

Institute involved in the work: PGI-1

Keywords: Magnetic skyrmions, Density Functional Theory (DFT),

Magnetic skyrmions are topologically protected, nanoscale spin textures char- acterized by a swirling configuration of magnetic moments. Their stability, small size, and efficient manipulation make them promising candidates for applications in data storage, spintronics, and quantum computing [1]. Their theoretical model- ing has largely relied on parameterized approaches, such as the extended Heisen- berg model, where parameters are derived from Density Functional Theory (DFT). However, the assumptions underlying these models—such as a constant magnetic moment—break down in complex configurations like Bloch points, highlighting the need for more accurate methods. The reliance on models has been due to computa- tional limitations that restricted DFT from treating large magnetic objects directly. However, advances in high-performance computing (HPC) and the GPU adapta- tion of the all-electron FLEUR code [2, 3, 4] have enabled precise, large-scale DFT simulations of skyrmions on exascale machines. These capture detailed magnetic and electronic properties—such as spatially varying magnetic moments and local densities of states—and allow direct calculation of energy barriers that determine skyrmion stability. [1] A. Fert et al., Nat. Rev. Mater. 2, 17031 (2017); A. Fert et al., Nat. Nanotechnol. 8, 152–156 (2013). [2] Jülich FLEUR Project, http://www.flapw.de [3] D. Wortmann et al., FLEUR, Zenodo (2023). https://doi.org/10.5281/zenodo.7576163 [4] E. Bosoni et al., Nat. Rev. Phys. 6, 45–58 (2024)

P-002 – Leveraging LLMs and ontologies for simulation data extraction and exploration

Elaheh Akhoundi

Authors: Elaheh Akhoundi, Stefan Sandfeld, Abril Azocar Guzman

Institute involved in the work: IAS-9

Keywords: Ontologies, materials science, large language models

The advent of data-driven approaches in materials science requires the aggregation of heterogeneous data from various sources, including simulation and experiments, which span different length scales and encompass a wide range of compositions, structures and thermodynamic conditions. While a vast amount of research data exists in materials science, much of it remains unstructured, limiting its reusability. Natural Language Processing (NLP) models like BERT, and large language models (LLMs) provide a solution for automating information extraction and database creation. However, making these tools applicable to materials science often requires adjustments for domain-specific tasks. This process can include preprocessing to structure research data, interacting with the LLM (including fine-tuning if needed), and postprocessing the extracted information. A way to ensure the quality and correctness of the extracted data is by the use of domain ontologies, which allows the alignment with the FAIR [1] data principles and increasing AI-readiness. We develop application and domain-specific ontologies [2], such as the Computational Material Sample Ontology, Crystallographic Defects Ontology Suite, and Atomistic Simulation Methods Ontology. The combination of LLMs and ontologies enable standardized documentation and efficient management of complex research data, promoting better data analysis, reuse, and data-driven discoveries.

References

[1] Wilkinson, M., Dumontier, M., Aalbersberg, I. et al., Sci Data, 2016, 3, 160018. [2] https://github.com/OCDO/

P-003 – CNN-based classification model for automated magnetic state identification in spin dynamics simulations

Amal Aldarawsheh, PGI-1

Authors: Amal Aldarawsheh, Ahmed Alia, Samir Lounis, Stefan Bluegel

Institute involved in the work: PGI-1 , IAS-7

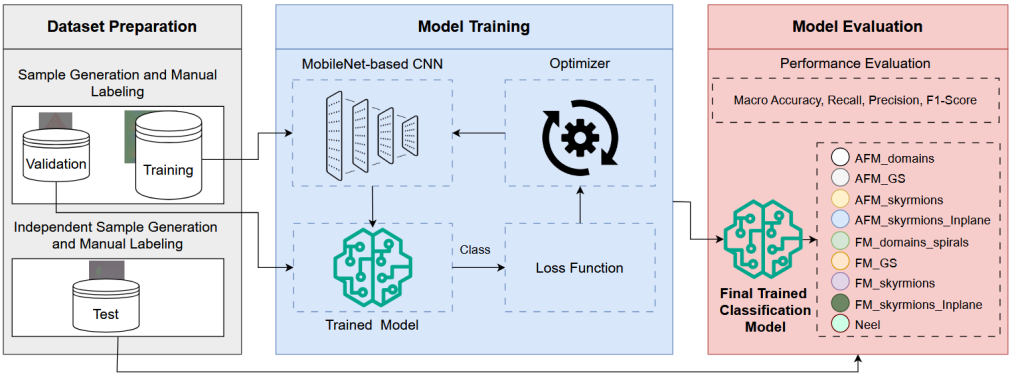
Keywords: AI, DL, CNN, Atomistic spin dynamics, classifications

The identification and classification of magnetic states emerging from atomistic spin dynamics simulations are essential for understanding complex magnetic behavior. While analytical scripts or handcrafted functions based on physical observables can be used, this approach often falls short for subtle or nontrivial spin textures. In many cases, ambiguities necessitate human visual inspection of spin configurations to confirm the magnetic state. This process is time- consuming, labor-intensive, and prone to error—particularly when analyzing large datasets. Therefore, there is a pressing need for automated solutions.

This work introduces a fully automated deep learning-based classification model for magnetic state identification. Leveraging the efficiency of Convolutional Neural Networks (CNNs) in feature extraction, we adopt a MobileNet-based CNN to encode spin configuration data. The extracted features are passed to a fully connected layer with a softmax activation function for classification into nine predefined magnetic states (see Figure 1).

To train and evaluate the model, we constructed a labeled image dataset where each image represents a spin configuration generated using the Spirit atomistic spin dynamics code and visualized via a customized VFRendering script. Each image was manually labeled according to its magnetic state. The dataset was randomly divided into training and validation sets. To ensure robust evaluation, an independent test set—generated with different magnetic interaction parameters—was used, preventing overlap with training or validation data. This setup enables an unbiased assessment of performance.

The results demonstrate that the MobileNet-based CNN model achieved 97% accuracy and F1-score, marking a significant step toward full automation of the *Spirit* workflow.



P-004 – Vision AI for Crowd Analysis

Ahmed Alia, Juelich Research Center, Institute for Advanced Simulation

Authors: Ahmed Alia

Institute involved in the work: IAS-7

Keywords: Artificial Intelligence, Deep Learning, Crowd Analysis, Pushing Behaviour Detection, Pedestrian Head Detection, Benchmark Dataset, Convolutional Neural Networks

AI-based video analysis has significantly improved the ability to understand crowd dynamics, which is crucial for effective crowd management and improving public safety. Crowd video analysis includes key tasks such as density estimation, counting, pedestrian trajectory extraction, and behavior detection. This abstract presents three Vision AI-driven projects initiated and developed at IAS-7: two focused on pushing behavior detection, and one aimed at supporting broader crowd analysis tasks.

The first project introduces a deep learning approach for localizing individuals involved in pushing behavior in recorded crowd videos [1]. Its goal is to support understanding the causes and risks of such behavior. Experiments demonstrate that the approach achieved an accuracy of 85%. As this approach does not meet real-time requirements, the second project addresses this gap by presenting a cloud-based deep learning system that detects pushing behavior in live video streams [2]. This enables timely alerts and supports early intervention by organizers and security personnel to prevent escalation. The real-time system achieved an accuracy of 86%.

The third project introduces a novel benchmark designed to support the development of efficient AI applications for various crowd analysis tasks in dense, high-risk environments such as railway platforms and event entrances [3]. It features a diverse dataset of 109,913 manually annotated, tailored explicitly for head detection in crowded scenes. The benchmark includes empirical evaluations of eight advanced deep learning models. Results show that You Only Look Once version 9 (YOLOv9) and Real-Time Detection Transformer (RT-DETR) achieved mean average precisions of 90.7% and 90.8%, respectively.

References

[1] Alia, Ahmed, Mohammed Maree, Mohcine Chraibi, and Armin Seyfried. “A novel Voronoi-based convolutional neural network framework for pushing person detection in crowd videos.” Complex & Intelligent Systems, 10(4), 2024, pp. 5005–5031. [2] Alia, Ahmed, Mohammed Maree, Mohcine Chraibi, Anas Toma, and Armin Seyfried. “A cloud-based deep learning framework for early detection of pushing at crowded event entrances.” IEEE Access, 11, 2023, pp. 45936–45949. [3] Abubaker, Mohamad, Zubayda Alsadder, Hamed Abdelhaq, Maik Boltes, and Ahmed Alia. “RPEE-HEADS: A Novel Benchmark for Pedestrian Head Detection in Crowd Videos.” arXiv preprint arXiv:2411.18164, 2024.

P-005 – Fire Dynamics Research: Multi-scale Experiments and Modeling for Fire Safety in the Build Environment

Lukas Arnold

Authors: Lukas Arnold

Institute involved in the work: IAS-7 , IET-4, JSC

Keywords: fire dynamics, civil safety, smoke dynamics, pyrolysis, CFD

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

Our research focuses on advancing fire safety through detailed multi- scale experiments, innovative numerical method development, and large- scale simulations utilizing high-performance computing (HPC) resources. Computational fluid dynamics (CFD) methods are essential in modeling fire and smoke spread within buildings. They enable increasingly precise geometric and phenomenological representations but present significant computational challenges due to complex multi- scale processes. Established in 2012 within the “Civil Safety and Traffic” division at the Jülich Supercomputing Centre and in collaboration with Bergische Universität Wuppertal (Chair for “Computational Civil Engineering”), the Fire Dynamics Group emphasizes developing and validating robust fire dynamics models and methods. Our contributions include freely accessible software, data sets, and advanced theoretical frameworks. One critical aspect we explore is the compromised visibility of evacuation signage during fires. Through real-scale fire experiments and theoretical model development, we investigate light-smoke interactions and human perception, enhancing the accuracy and realism of CFD simulations and virtual reality (VR) smoke representations. Predicting fire initiation and propagation accurately remains a significant challenge. Our micro-scale experiments investigate material pyrolysis to determine precise parameters used in CFD modeling, ultimately improving large-scale flame spread predictions, aiding in fire prevention strategies, and supporting safer evacuation protocols.

P-006 – Active Matter in Alignment Fields

Thorsten Auth, Forschungszentrum Jülich

Authors: Sameh Othman, Gerhard Gompper, Jiarul Midya, Thorsten Auth

Institute involved in the work: IAS-2

Keywords: Active Matter, Active Brownian Particles, aligned motion, confined geometries, cooperative interaction.

Active Brownian particles (ABPs) are self-propelled colloids that display intriguing collective behaviors, such as motility-induced phase separation. Previously, we have studied the phase behaviour of ABPs subject to thermal noise, a self-propulsion velocity, and a homogeneous alignment field for the self-propulsion velocity. Here, we characterize the flow of aligned ABPs in complex channel geometries. For branched channels with Y, T, and inverted Y-geometries, which are overall oriented parallel to the direction of the field, non-interacting ABPs move fastest in channel sections oriented parallel to the alignment field. In channel sections tilted with respect to the field, the ABP velocities are reduced. For inverted-Y-channels, where particles in titled channel segments have to flow opposite to the field direction, the cooperative interaction between ABPs significantly increases the flow compared to non- interacting ABPs. To elucidate these findings, we quantify the local ABP densities and flow velocities along the channel. Our analysis allows for the prediction of the parameters to maximise the flow of aligned self-propelled particles in complex geometries.

References

Sameh Othman, Jiarul Midya, Thorsten Auth, and Gerhard Gompper. Phase behavior and dynamics of active brownian particles in an alignment field. Physical Review E, 111(1), January 2025
http://dx.doi.org/10.1103/PhysRevE.111.015425

Acknowledgements

We gratefully acknowledge computing time on the supercomputer JURECA at Forschungszentrum Jülich under grant no. cjiff26. SO thanks the Palestinian German Science Bridge for financial support.

P-007 – exacb: A Template-Based Framework for Continuously Benchmarking on Exascale Systems

Jayesh Badwaik, Forschungszentrum Juelich

Authors: Andreas Herten, Jayesh Badwaik, Mathis Bode

Institute involved in the work: JSC

Keywords: exascale, continuous benchmarking, jureap, early access

exaCB is a framework designed to automate and standardize Continuous Integration (CI) and Continuous Benchmarking (CB) for HPC applications. By offering a template-based infrastructure, it allows users to define and execute benchmarks in a declarative, key-value-based manner. This approach ensures well-defined workflows aligned with best practices, while integrated automated data analytics streamlines performance monitoring and energy usage tracking with minimal user input. The consistent workflow structure enables faster turnaround times, allowing users to efficiently adapt to various changes, such as resource management configurations, software updates, or the deployment of new experimental setups.

Currently, exaCB is used and further developed within the context of JUPITER, JEDI, and JUPITER Research and Early Access Program (JUREAP) with over 100 applications, where it serves as a core tool for performance enablement, assessment, and monitoring. Although its design is agnostic to specific benchmarking frameworks and CI backends, it has primarily been tested on JSC systems using EasyBuild, GitLab CI/CD, and JUBE scripts. We are exploring opportunities to extend exaCB's use to other systems and workflows, aiming to broaden its applicability and enhance its flexibility across various HPC environments as well as other application-based workflows.

P-008 – Diffusion Model for Scientific Image Reconstruction

Arya Bangun, Forschungszentrum Jülich

Authors: Laurentius Valdy, Richard Paul, Alessio Quercia, Zhuo Cao, Hanno Scharr, Arya Bangun

Institute involved in the work: IAS-8

Keywords: Diffusion Model, Image Reconstruction, STEM, MRI

Diffusion models have emerged as powerful tools for generating both 2D and 3D images, achieving significant success in computer vision, data augmentation, and image and video generation. These models excel at capturing complex data distributions and producing high-fidelity images by iteratively refining random noise into coherent structures. Despite their success with natural images, applying diffusion models to scientific imaging remains challenging due to the unique characteristics of specialized modalities such as microscopy, spectroscopy, and medical imaging. Additionally, scientific image reconstruction often requires transforming raw measurement data into a meaningful representation of the object under investigation. We propose a framework that integrates diffusion models with reconstruction algorithms to enhance the quality of scientific imaging. Our approach demonstrates improved reconstruction performance in applications such as Magnetic Resonance Imaging (MRI) and Scanning Transmission Electron Microscopy (STEM).

P-009 – Performance Portability across GPU vendors and Programming Models

Rodrigo Bartolomeu, FZJ

Authors: Godehard Sutmann, Jan H. Meinke, René Halver, Rodrigo Bartolomeu

Institute involved in the work: JSC

Keywords: Performance Portability; GPU; Programming Models; High Performance Computing; N-Body problem

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

The accelerated HPC landscape has changed significantly in recent years, creating new challenges for scientific code developers. Initially, Nvidia was the primary provider of GPGPUs for such systems. Most Tier 1 supercomputers required the adoption of CUDA in order to write code that could properly explore the compute capabilities of the accelerators. In recent years, however, other vendors such as AMD and Intel have taken up the hardware development. As of November 2024, the top 10 in the top 500 list have systems with hardware from all three major vendors. Maintaining entire code bases that run on multiple architectures is now highly desirable and time-consuming. Since each vendor provides its own preferred programming models for its hardware, it becomes relevant to compare the portability of these models across hardware platforms. For this work, we have implemented the N-body problem with different optimizations using native and portable programming frameworks. We will share our experiences and present the results of our recent study using the same code for the N-body problem on four different architectures from the three major vendors: Nvidia's GH200 and A100, AMD's MI250, and Intel's GPU MAX 1100 in seven programming models.

P-010 – Adhesion-driven translocation of vesicles through membrane-covered pores

Nishant Baruah, Forschungszentrum Jülich

Authors: Nishant Baruah, Jiarul Midya, Gerhard Gompper, Anil Kumar Dasanna, Thorsten Auth

Institute involved in the work: IAS-2

Keywords: Pore translocation, parasite-host invasion, continuum membrane model, vesicles

Apicomplexan parasites like Plasmodium, which transmits malaria, invade host cells by translocating through a tight junction at the host plasma membrane. This process presents significant physical challenges, including the need for the parasite to deform its own membrane while squeezing through the tight junction and contending with the host membrane tension [1]. Vesicles are a well-established biophysical model system that possibly provides insights into Apicomplexan invasion mechanisms.

In this study, we investigate the translocation of vesicles through membrane-covered pores driven by an energy gain through contact adhesion [2]. We use continuum models for both, vesicles and membranes, and perform the calculations using energy minimization on the discretized triangulated membranes. This allows us to predict stable translocation states for various vesicle- and host-membrane elastic properties and vesicle-to-pore size ratios. The strong particle deformation upon pore translocation results in an energy barrier which needs to be overcome to access the deep-translocated states. For prolate vesicles, the energy barrier can be significantly reduced compared to initially spherical vesicles, but the translocation can be entirely suppressed if the vesicle membrane area is too small to enclose its volume at half-wrapping. We also observe that a finite-host membrane tension strongly suppresses pore translocation, which may explain protection against severe malaria in the Dantu blood group [3].

References

[1] S. Dasgupta et al, Biophys. J. 107, 43 (2014).

[2] N. Baruah et al., Biophys. J. 124, 5 (2025).

[3] S. N. Kariuki et al, Nature 585, 579 (2020).

Acknowledgements

NB, AKD, and TA acknowledge funding by the DFG SPP 2332 ”Physics of Parasitism”, and helpful discussions with Mirko Singer (Heidelberg), and Javier Periz and Markus Meissner (Munich).

P-011 – Algorithms, Tools and Methods Lab Advanced Time Integrators

Thomas Baumann, Forschungszentrum Juelich

Authors: Abdelouahed Ouardghi, Jannik Finck, Mehdi Babamehdi, Robert Speck, Ruth Partzsch, Simon Wenchel, Sriramkrishnan Muralikrishnan, Thomas Baumann

Institute involved in the work: JSC

Keywords: PDEs, HPC, parallel-in-time, parallel-in-space, particle-in-cell, CFD

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

The Algorithms, Tools and Methods Lab Advanced Time Integrators (ATML ATI) is a group at JSC researching mathematics around time-dependent differential equations in the context of high-performance computing (HPC). We work on novel time-integration methods and their properties, including parallelization in time, adaptivity, resilience, well as their interplay with space-parallel approaches. We also focus on the efficient implementation of these methods tailored to modern HPC machines and demonstrate speedup for practical applications such as particle-in-cell plasma simulations and finite-element fluid dynamics simulations. Our research software is publicly accessible via the open-source codes IPPL and pySDC, which we develop and maintain. Beyond our research, we are involved in software support for the HPC systems and are always open for collaborations, such as implementing time-parallel methods in application codes or prototyping methods of interest.

P-012 – No more shots in the dark - Highly efficient compression basis for live ptychography

Paul F. Baumeister, Jülich Supercomputing Centre

Authors: Paul F. Baumeister, Alexander Clausen, Arya Bangun, Dieter Weber

Institute involved in the work: Other , JSC

Keywords: electron microscopy, data compression, live processing, imaging data

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

The field of electron microscopy (EM) will soon be a hundred years old. However, advances in abberration correction have improved transmission EM during the last two decades. Single atoms can now become visible. We can move the electron beam focus over a sample to get scanning transmission electron microscopy (STEM) data. Then, a 2D-array of scan points come in sequentially, while each scan point is a 2D diffraction image, hence are called 4D-STEM data sets. The Wigner distribution deconvolution method (WDD) allows to visualize a real-space representation of the sample. However, WDD with full images is costly and has so far been performed as a postprocessing step only. A viable alternative is data compression on the diffraction images. Various methods of dimensionality reduction have been tried. Our approach is to use the circular harmonic oscillator (CHO) basis for three reasons: (1) The CHO basis has been found to be highly efficient in compressing typical 2D diffraction images while suppressing statistical noise. (2) The factorizable property of the Cartesian representation of a CHO basis allow for CHO basis transformations using a two-step scheme of efficient matrix-matrix multiplication SGEMM. (3) The WDD procedure can skip two Fourier transforms due to an analytical property of the CHO basis. Combining the three aspects of acceleration LiberTEM-live can visualize 4D-STEM data using CHO-WDD in milliseconds on a GPU, even on incomplete scans. This allows EM operators to finally see what they measure while the scan is still running.

References

https://academic.oup.com/mam/article/29/3/994/7072677

P-013 – Leveraging Experimental Vasculature Data for High Resolution Brain Tumor Simulations

Eric Behle, Forschungszentrum Jülich

Authors: Eric Behle, Julian Herold, Alexander Schug

Institute involved in the work: JSC , Steinbuch Centre for Computing, Karlsruhe Institute of Technology

Keywords: Tumor simulation, mouse brain, vasculature

Cancer remains a leading cause of mortality. Multidisciplinary studies probe its complex pathology to increase treatment options. Computational modeling of tumor growth on high-performance computing resources offers microscopic insight into its progress and a valuable avenue for advancing our understanding. However, the effective initialization and parameterization of the underlying mod- els require high-resolution data from real tissue structures. Here, we leveraged high performance computing resources and a massive dataset of a mouse brain's entire vascular network. We processed these image stacks into detailed three- dimensional representations, identified brain regions of interest, and conducted a series of large-scale simulations to investigate how tumor growth is influenced by local vascular network characteristics. By simulating tumor growth with sub- cellular resolution, we can probe to which extent vessel density and vessel network length influence tumor growth. We determined that vessel density is the primary determinant of growth rate. Finally, our results allowed us to extrapolate tumor cell growth predictions for the entire mouse brain, highlighting the critical role of vascular topology in tumor progression. Such increasingly realistic simulations of cancer cells and their microenvironment enable researchers to increasingly bridge the gap between basic biology and clinical practice, ultimately supporting the development of more effective personalized cancer therapies.

P-014 – Porting the hydrologic model ParFlow to different accelerator architectures using eDSL and Kokkos

Joerg Benke

Authors: Joerg Benke, Muhammad Fahad, Andreas Herten, Daniel Caviedes Voullieme, Stefan Kollet

Institute involved in the work: JSC , IBG3 (also main contributor)

Keywords: Hydrologic Model, Domain Specific Language, GPU Porting, Kokkos, Cuda/HIP

The ParFlow hydrologic model is an integrated variably saturated groundwater, surface water flow simulator that incorporates subsurface energy transport and land surface processes. ParFlow has been coupled to different atmospheric models and is also integrated in the German climate and weather prediction ICON(-Land) software ecosystem and the Terrestrial Systems Modeling Platform (TSMP).

ParFlow is mainly written in C and uses the parallelization methods MPI, OpenMP, native CUDA support and the programming model Kokkos (with the backend CUDA, HIP or OpenMP). The parallelism in ParFlow has been abstracted early on in what is called an embedded Domain Specific Language (eDSL) which is leading to a best-practice separation-of- concerns and abstracts away implementation details.

Since future hardware will be characterized by varying architectures there was a demand to also enable HIP for AMD architectures (e.g. the pre-exascale HPC system LUMI of EuroHPC). To implement HIP for ParFlow via the eDSL and Kokkos the porting work was started in the national Earth System Modelling Initiative (natESM at JSC) and was finished at IBG3 (Forschungszentrum Jülich) which resulted in a high degree of performance portability.

In this poster we will present the eDSL of ParFlow and also how Kokkos (with the Cuda and HIP backend) is included in the eDSL and to allow ParFlow to reach performance portability on the basis of the eDSL and Kokkos with the change of only a limited amount of lines. Scalability plots of ParFlow on JUWELS Booster (Nvidia A100 GPUS) and LUMI (Finland) with AMD MI250X accelerators are presented.

P-015 – JAIF - The JUPITER AI Factory

Mathis Bode, Forschungszentrum Jülich GmbH

Authors: Kristel Michielsen, Mathis Bode, Thomas Lippert

Institute involved in the work: JSC

Keywords: AI, JUPITER

The AI Factories play a key role in the European science ecosystem. Currently, a new AI Factory, the JUPITER AI Factory (JAIF), is established with the first European exascale supercomputer JUPITER at its center. This poster gives an outlook at the JAIF ecosystem.

P-016 – JUREAP - The JUPITER Research and Early Access Program

Mathis Bode, Forschungszentrum Jülich GmbH

Authors: Mathis Bode, Andreas Herten, Benedikt von St. Vieth, Jayesh Badwaik, Wolfgang Frings

Institute involved in the work: JSC

Keywords: Exascale

JUPITER will be the first Exascale supercomputer in Europe. JUREAP, the JUPITER Research and Early Access Program, plays a key role in successfully bringing JUPITER into full production and enabling groundbreaking new science. This poster presents the workflows and early results.

P-017 – 3D Motion in Crowds

Maik Boltes, Forschungszentrum Jülich

Authors: Ann Katrin Boomers, Carina Wings, Deniz Kilic, Juliane Adrian, Maik Boltes, Sina Feldmann

Institute involved in the work: IAS-7

Keywords: Pedestrian Dynamics, Crowd, 3D Motion Capturing

For understanding the dynamics inside crowds, reliable empirical data are needed, which could increase safety and comfort for pedestrians and the design of models reflecting the real dynamics.

In dense crowds a well-calibrated camera system can extract absolute head positions with high accuracy. The inclusion of inertial sensors or even self-contained full-body motion capturing systems allows the relative tracking of body parts or even capturing the locomotion of the whole body. To capture the 3D motion of people inside a crowd relative to surrounding people movement data of both systems have to be fused.

To analyze effects like clogging, overtaking or the threading into a bottleneck the orientation and with this the space usage of body parts like shoulder, pelvis, arms and feet are of high interest. Other research using the 3D motion of body parts is looking at the movement adaptations as a reason for injury risks or how pushes are propagated through a crowd.

References

Boomers Ann Katrin, Maik Boltes, and Uwe G. Kersting. “How Approaching Angle, Bottleneck Width and Walking Speed Affect the Use of a Bottleneck by Individuals.” Sensors 24, no. 6. 2024: 1720. https://doi.org/10.3390/s24061720. Feldmann Sina, Thomas Chatagnon, Juliane Adrian, Julien Pettré, and Armin Seyfried. “Temporal Segmentation of Motion Propagation in Response to an External Impulse.” Safety Science 175. 2024: 106512. https://doi.org/10.1016/j.ssci.2024.106512. Feldmann Sina, Juliane Adrian, and Maik Boltes. “Propagation of Controlled Frontward Impulses Through Standing Crowds.” Collective Dynamics 9. 2024. https://doi.org/10.17815/CD.2024.148. Feldmann Sina, and Juliane Adrian. “Forward Propagation of a Push through a Row of People.” Safety Science 164. 2023: 106173. https://doi.org/10.1016/j.ssci.2023.106173. Boomers Ann Katrin, and Maik Boltes. “Shoulder Rotation Measurement in Camera and 3D Motion Capturing Data.” In Traffic and Granular Flow ’22, 35–42. 2024. https://doi.org/10.1007/978-981-99-7976-9_5. Boltes Maik, Juliane Adrian and Anna-Katharina Raytarowski. “A Hybrid Tracking System of Full-Body Motion Inside Crowds.” Sensors 2021, 21(6), 2108, https://doi.org/10.3390/s21062108.

P-018 – Phonons in FLEUR employing Density Functional Perturbation Theory

Thomas Bornhake, Forschungszentrum Jülich

Authors: Thomas Bornhake, Alexander Neukirchen, Daniel Wortmann, Gregor Michalicek, Gustav Bihlmayer, Stefan Blügel

Institute involved in the work: PGI-1

Keywords: DFT, FLAPW, Phononen, DFPT

Phonons are significant for various physical properties and phenomena, such as instabilities and spin-flip scattering. Their incorporation into materials design has increased, necessitating an efficient method for calculating phonons under diverse excitations. In this poster, we present the successful implementation of state-of-the-art Density Functional Perturbation Theory (DFPT) within the all-electron full- potential linearized augmented plane-wave (FLAPW) method, FLEUR [1,2]. We benchmark our method against experimental data for both magnetic and non-magnetic systems. Additionally, we discuss our progress in extending the method to model thin-film systems efficiently in semi- infinite vacuum [3], as well as guiding the way for predicting superconducting transition temperatures.

References

[1] D. Wortmann et al., 10.5281/zenodo.7576163; www.flapw.de [2] C.-R. Gerhorst et al., Electron. Struct. 6, 017001 (2024) [3] H. Krakauer et al., Phys. Rev. B 19, 1706 (1979)

P-019 – Using normalizing flows to investigate neural manifold properties and curvatures.

Peter Bouss

Authors: Alexandre Rene, Kirsten Fischer, Moritz Helias, Peter Bouss, Sandra Nestler

Institute involved in the work: IAS-6 , (1) Institute for Advanced Simulation (IAS-6), Jülich Research Centre, Jülich, Germany (2) RWTH Aachen University, Aachen, Germany (3) Rappaport Faculty of Medicine and Network Biology Research Laboratory, Technion - Israel Institute of Technology, Haifa, Israel (4) Department of Physics, Faculty 1, RWTH Aachen University, Aachen, Germany (5) International School of Advanced Studies (SISSA), Trieste, Italy (6) Department of Physics, University of Ottawa, Ottawa, Canada (7) Department of Computer Science, RWTH Aachen University, Aachen, Germany

Keywords: Normalizing Flows

Despite the large number of active neurons, neuronal population activity appears to occur on low-dimensional manifolds (Gallego et al., 2017). Variants of principal component analysis are frequently used to evaluate this manifold, neglecting higher-order cumulants.

We employ Normalizing Flows (NFs) to learn brain activity statistics without making such major assumptions. These neural networks are trained to estimate a probability distribution by learning a map from a latent distribution, that we select to be a Gaussian mixture.

We change NF's training objectives to distinguish between meaningful and noisy dimensions. We ensure this using a stacked dropout approach in the latent space (Bekasov & Murray, 2020). By approximating the network for each mixed component as a quadratic mapping, we can determine the neural manifold's Riemannian curvature tensors.

Finally, the method is applied to electrophysiological recordings of the macaque visual cortex (Chen et al., 2022). Morales-Gregorio et al., 2024 showed that these data lie on two distinct manifolds. We demonstrate that the shapes of the manifolds differ decisively from a flat space. Analyzing the curvature of the manifolds provides insights into the regimes in which neuron groups interact non-linearly.

P-020 – Preparing for Exascale with BigDays

Thomas Breuer *and*

Wolfgang Frings

Authors: Filipe Guimaraes, Jolanta Zjupa, Oliver Mirus, Thomas Breuer, Wolfgang Frings

Institute involved in the work: JSC

Keywords: BigDays, HPC, Supercomputing, Exascale

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

As HPC moves towards exascale computing, balancing large-scale scientific workflows within daily production remains challenging. Simply scheduling large-scale runs in the same queue as other jobs leads to long queue waiting times for all users on the HPC system, and to overproportional loss of compute resources during the draining phase that precedes every large-scale run. To address this, we introduce a concept called BigDays: special, regularly scheduled reservations dedicated to (near) full-system workloads enabling scientists to explore performance limits, optimise applications, and mimic exascale scenarios without incurring excessive scheduling overhead. In this poster, we detail the implementation of the BigDays at the Jülich Supercomputing Centre (JSC) and how it demands close coordination among users, support teams, and system administrators. In addition, we show a first evaluation of the gathered system and usage data from over 15 BigDays in six months in 2024, with a total of 1,217 jobs from 36 different projects with various usage models: scaling tests, large-scale debugging, production, and AI workflows. By consolidating (near) full-system usage into defined intervals, we not only reduce system fragmentation and the impact on regular production but also accelerate application readiness for exascale.

P-021 – JSC HPC User Support and Services

Filipe Guimaraes, Jülich Supercomputing Centre *and*

Thomas Breuer *and*

Wolfgang Frings

Authors: Filipe Guimaraes, Thomas Breuer, Wolfgang Frings

Institute involved in the work: JSC

Keywords: HPC, Support, User Service, Supercomputing

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

The primary mission of cross-domain Algorithms, Tools and Methods Labs - Application Optimisation and User Service Tools (ATML-AO) is HPC user support on the JSC supercomputing systems. We provide support through three major channels: direct on-demand and proactive user support through the ticket system as a service, the development and maintenance of open-source HPC tools, as well as training in form of courses on HPC topics. In this poster, we will present an overview of the above topics in order to have a direct exchange with IAS HPC users about our services.

P-022 – Mastering HPC monitoring data: from zero to hero with LLview

Filipe Guimaraes, Jülich Supercomputing Centre *and*

Thomas Breuer *and*

Wolfgang Frings

Authors: Filipe Guimaraes, Thomas Breuer, Wolfgang Frings

Institute involved in the work: JSC

Keywords: hpc, supercomputing, monitoring, operational data analytics

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

Monitoring jobs in large high-performance computing systems requires careful attention to misconfigurations, system errors, inefficient resource usage, and missed optimisation opportunities. Although users are best placed to spot these issues, they may lack the necessary knowledge, interest, or permissions often shift this responsibility to operational teams, who face the challenging task of overseeing a diverse workload alongside other pressing duties. In this poster, we present LLview, an open-source tool that gathers metrics from various monitoring sources and delivers processed data and analysis through a clear, role-based web portal. LLview is used on all production systems at the Jülich Supercomputing Centre, providing relevant information to users, project leaders, mentors, and support personnel. The job and system data offered by LLview help both users and support teams improve supercomputer usage and quickly address issues. LLview has been further developed as part of several projects, including SiveGCS (NRW), DEEP-SEA, IO-SEA, and EUPEX (EU). With its open-source release, we also hope to collaborate with other HPC centres worldwide.

P-023 – Spiking neural networks for controlling a biomechanically realistic arm model

Philip Bröhl, IAS-8 / IAS-6

Authors: Philip Bröhl, Ira Assent, Junji Ito, Sonja Grün

Institute involved in the work: IAS-6 , IAS-8

Keywords: Motor Cortex Model, System Dynamics, System Behaviour, Network Properties

POF Topic: P2T3: Neuromorphic Computing and Network Dynamics

A typical feature of neurons in the motor cortex of mammalian brains is that they are tuned to a particular direction of movements, i.e. they exhibit most spikes when a body part is moved in a particular direction, called preferred direction (PD). It has been reported that the distribution of preferred directions among motor cortex neurons depends on the constraints in the movements: when the arm may move freely in 3D, it is uniform [1,2], but when it is constrained to a 2D movement, it is bimodal [3,4].

In this project, we aim at revealing the neuronal mechanism underlying the emergence of a bimodal PD distribution, by studying an artificial network of spiking neurons. Our model is implemented in Tensorflow [5] and consists of 300 recurrent leaky integrate-and-fire neurons with 6 linear readout neurons that control the 6 muscles in a biomechanical arm model [4]. We train it to output muscle activation signals to perform a 2D reaching task. After training, the recurrent neurons show directional tuning with bimodally distributed PDs.

Our next steps are to further study and compare the model behavior to experimental findings. Therefore, we elucidate: a) Are neurons in the SNN tuned to muscle commands rather than directions in the movement space, b) does that explain the bimodal distribution of preferred hand movement directions, c) when the model performs sequences of movements as in the experiment, does the model show specific spatio-temporal patterns of spikes?

References

1. Caminiti, R., Johnson, P. B., & Urbano, A. (1990). Making arm movements within different parts of space: Dynamic aspects in the primate motor cortex. Journal of Neuroscience, 10(7), 2039–2058. https://doi.org/10.1523/JNEUROSCI.10-07-02039.1990 2. Schwartz, A. B., Kettner, R. E., & Georgopoulos, A. P. (1988). Primate motor cortex and free arm movements to visual targets in three-dimensional space. I. Relations between single cell discharge and direction of movement. The Journal of Neuroscience: The Official Journal of the Society for Neuroscience, 8(8), 2913–2927. https://doi.org/10.1523/JNEUROSCI.08-08-02913.1988 3. Lillicrap, T. P., & Scott, S. H. (2013). Preference Distributions of Primary Motor Cortex Neu-rons Reflect Control Solutions Optimized for Limb Biomechanics. Neuron, 77(1), 168–179. https://doi.org/10.1016/j.neuron.2012.10.041 4. Codol, O., Michaels, J. A., Kashefi, M., Pruszynski, J. A., & Gribble, P. L. (2024). MotorNet: A Python toolbox for controlling differentiable biomechanical effectors with artificial neural networks. eLife, 12. https://doi.org/10.7554/eLife.88591.3 5. TensorFlow Developers. (2025). TensorFlow. Zenodo. https://doi.org/10.5281/zenodo.4724125

Acknowledgements

This work was partially performed as part of the Helmholtz School for Data Science in Life, Earth and Energy (HDS-LEE) and received funding from the Helmholtz Association of German Research Centres. This research was partially funded by the NRW-network 'iBehave', grant number: NW21-049.

P-024 – Inbound licensing with ease

Dirk Brömmel

Authors: Dirk Brömmel, Robert Speck

Institute involved in the work: JSC

Keywords: JuRSE RSE GitLab

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

Managing projects with external collaborators sometimes comes with the burden of ensuring inbound contributions respect legal obligations. Where a low-level ‘Developer Certificate of Origin (DCO)’ approach only introduces certain checks, a ‘Contributor License Agreements (CLAs)’, on the other hand, relies on documenting signed CLAs and thus dedicated book-keeping. In this poster, we showcase our initial approach to a ‘CLA Bot’ that checks merge requests on compliance with either a DCO or CLA. While this is work in progress, our goal is to provide a similar functionality already available on Github also for community instances of Gitlab. We show the interaction between the bot and users, its limitations, and list steps taken for the automation via CI pipelines. Here, the somewhat simpler approach to pipelines in Gitlab vs Github necessitates working with webhooks that act on events within Gitlab. Our setup does not rely on a central server (in fact any additional server) and can be used by individual projects without having to share data. By using webhooks and CI pipelines, our approach can be used for similar automation tasks, offering the potential to interact with users.

P-025 – Simulation and Data Lab Terrestrial Systems

Daniel Caviedes Voullieme, Forschungszentrum Jülich

Authors: Daniel Caviedes Voullieme, Ana Gonzalez-Nicolas, Stefan Poll, Joerg Benke, Paul Rigor

Institute involved in the work: JSC , IBG-3

Keywords: Terrestrial Systems, Hydrology, HPC, Exascale

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

The Simulation and Data Lab Terrestrial Systems (SDLTS) focuses on numerical simulation of terrestrial system and ecohydrological processes across scales, leveraging and the pushing the limits of high-performance computing and scientific software.

Global change is affecting terrestrial systems at all scales. It results in major changes of the land surface and ecosystems and of the services provided by them with several socioeconomic impacts. Many processes are still poorly understood or reproduced by models.

HPC simulations are central to terrestrial systems research, providing insights about system processes and information for sustainable management of terrestrial systems. In particular SDLTS explores complex, nonlinear transport of energy, mass and momentum; interactions and feedback mechanisms between different compartments of the coupled geo-eco-hydro system (subsurface, land-surface, atmosphere, reservoirs) at multiple spatio-temporal scales, and high resolutions; and environmental hydrodynamics. Our work spans from catchment to regional Earth system scales, thus interacting with small scale processes all the way to climate scales.

SDLTS is also involved in exascale readiness at JSC, investing strongly on performance-portability, heterogeneous and modular supercomputing approaches.

P-026 – IAS-7 : Crowd Simulation and Analysis Softwares

Thomas Chatagnon, IAS-7

Authors: Mohcine Chraibi, Thomas Chatagnon

Institute involved in the work: IAS-7

Keywords: Crowd Modeling, Python, Open Source, Analysis library

We would like to propose an overview of the two main open source software developed and used in the IAS-7 Modelling Division. The first software, *JuPedSim*, is a crowd simulation platform. It couples a C++ core to a Python API, allowing users to easily implement computationally efficient crowd simulations. The second software, *PedPy*, is a Python library for crowd analysis. This open source library provides a set of convenient plotting and analysis functions to study simulated or experimentally collected pedestrian trajectories.

P-027 – Temperature dependent quadratization from 3SAT to QUBO

Alexandru Ciobanu, forschungszentrum Julich

Authors: Alexandru Ciobanu, David Dahmen, Moritz Helias

Institute involved in the work: IAS-6

Keywords: Monte Carlo Sampling, Glauber Dynamics, 3-SAT, Ising model, combinatorial optimization, statistical physics, thermal energy, QUBO, partition function.

POF Topic: P2T3: Neuromorphic Computing and Network Dynamics

Combinatorial optimization has widespread application: in resource allocation, routing, cryptography, or genetics. These problems can be traced back to a universal optimization problem, K-satisfiability (K-SAT), which searches for words of N boolean variables that adhere to a set of logical or clauses. It has been shown that this problem is NP complete as soon as three (3-SAT) or more variables are combined in a clause.

We study this problem starting from its known mapping to the ground state of a classical spin Hamiltonian with third order interactions. This statistical physics approach prepares an equilibrium distribution of variables with thermal energy given by β^{-1}. The optimum is attained for $\beta \to \infty$, typically by Monte-Carlo sampling.

We derive a novel procedure to transform the 3-SAT Hamiltonian so that at most quadratic interactions appear (QUBO), while preserving the partition function. In this sense the transform implements a renormalization step. The transform comes at the expense of introducing additional variables. These extra variables, however, undergo a simple dynamics in the Monte-Carlo sampler (Glauber dynamics) that can be solved analyticaly and accounted for, again reducing the number of degrees of freedom to that of the original system. As a result, we find an efficient method to solve the 3-SAT optimization problem that only requires pairwise interactions, thus only requiring matrix-vector multiplications in the Monte-Carlo sampler while having the same performance as sampling from the original system. This reduction of interaction order may be decisive in enabling neuromorphic implementations of the solver.

P-028 – MExMeMo: Multi-Scale Polymer Digital Twin using Modular Supercomputing Architecture

Adel Dabah, JSC

Authors: Adel Dabah, Andreas Herten

Institute involved in the work: JSC

Keywords: Modular Supercomputing Architecture (MSA), GPU

The MExMeMo Project creates a digital twin for polymer optimization, validation, and fabrication by coupling GPU-accelerated particle dynamics models with continuum methods via the Modular Supercomputing Architecture (MSA). The particle dynamics model (SOMA) tracks individual elements in high detail but requires intensive computational resources (memory, processing power, and time), while the continuum method (UDM) sacrifices detail for computational efficiency and scalability, allowing coarse-grained simulations at large physical scales. JSC enables these coupled simulations through a coordinator framework for resource/data orchestration and in-depth hardware-specific performance optimizations. These optimizations allowed to double memory throughput in the SOMA application, boosting timesteps per second (TPS) by 2.2x, and cutting power consumption threefold. We also achieved a 30% reduction in execution time for the UDM code through GPU-specific optimizations, including kernel refactoring to reduce thread divergence, enhanced memory coalescing for efficient data access. These improvements will also boost the speedup of the coupled simulations, as the UDM model's performance is a critical bottleneck for the overall system. Future work will focus on further GPU kernel tuning and workload balancing to maximize scalability.

P-029 – Interaction of microgels with lipid membranes

Tanwi Debnath, Forschungszentrum Juelich

Authors: Tanwi Debnath, Jiarul Midya, Thorsten Auth, Gerhard Gompper

Institute involved in the work: IAS-2

Keywords: microgels, membranes, wrapping, bending rigidity, elasticity

POF Topic: P2T4: Molecular and Cellular Information Processing

The interaction of nano- and microcarriers with lipid-bilayer membranes plays a key role for cellular engulfment and drug delivery [1]. The physico-chemical parameters of the particles that control engulfment are their size, shape, and deformability [2]. Microgels are particularly versatile because their elasticity can be tuned in a wide range by changing the density of crosslinkers. Using an elastic- network model for the microgel and triangulated surfaces for the membrane, we study microgel wrapping at lipid-bilayers. We use the Hertz theory to characterize the microgel's Young's modulus and Poisson's ratio. We then determine the interplay of microgel and membrane deformation controlled by the competition between membrane bending rigidity and microgel elasticity. Our calculations predict an increased stability of partial-wrapped states for microgels with lower Young's moduli [3]. There is a discontinuous transition from oblate microgel shapes at low wrapping fractions to cup-like shapes at high wrapping fractions. At membranes with high tension, we also observe another discontinuous transition at deep-wrapped states between cup- like shapes of microgels and nearly spherical shapes [3]. Our results will allow the design of the microgels with optimal elastic properties for biomedical applications.

References

[1] S. Dasgupta, T. Auth and G. Gompper, J. Phys. Condens. Matter 29, 373003 (2017). [2] X. Liu et al., Proc. Natl. Acad. Sci. USA, 120, e2217534120 (2023). [3] T. Debnath, J. Midya, T. Auth and G. Gompper, in preparation, 2025.

Acknowledgements

SFB 985 Functional Microgels and Microgel Systems, Alexander von HUMBOLDT Foundation

P-030 – Bioplausible Contrastive Learning with a Linear Memory Chain

Nils Derner, Forschungszentrum Jülich

Authors: Nils Derner, Willem Wybo

Institute involved in the work: PGI-15

Keywords: local learning, self-supervised learning, long-timescale neural dynamics

POF Topic: P2T3: Neuromorphic Computing and Network Dynamics

strong textHow the brain achieves deep learning of rich and robust representations is still an open question. Artificial neural networks (ANNs) offer interesting approaches to this problem, as their architecture is often based on insights from neuroscience. However, in contrast to common ANNs, which use end-to-end backpropagation, labels, and batched data, biological neurons learn locally, primarily unsupervised, and online. While recent advances in self-supervised learning, such as contrastive learning, enable training without labels, these methods inherently require batched data. In our work, we developed a simple neuron-local memory mechanism in the form of a linear chain that enables online contrastive learning. We demonstrate that this linear memory chain, when combined with layer-local learning, builds robust representations that improve with layer depth and outperform state-of-the-art layer-local learning rules.

References

[1] Serin Atiani, Mounya Elhilali, Stephen V David, Jonathan B Fritz, and Shihab A Shamma. Task difficulty and performance induce diverse adaptive patterns in gain and shape of primary auditory cortical receptive fields. Neuron, 61(3):467–480, 2009. [2] Ting Chen, Simon Kornblith, Mohammad Norouzi, and Geoffrey Hinton. A simple framework for contrastive learning of visual representations. In International conference on machine learning, pages 1597–1607. PMLR, 2020. [3] Adam Coates, Andrew Ng, and Honglak Lee. An analysis of single-layer networks in unsupervised feature learning. In Proceedings of the fourteenth international conference on artificial intelligence and statistics, pages 215– 223. JMLR Workshop and Conference Proceedings, 2011. [4] Gail Gilboa, Ronen Chen, and Naama Brenner. History-dependent multiple-time-scale dynamics in a single-neuron model. Journal of Neu- roscience, 25(28):6479–6489, 2005. [5] Manu Srinath Halvagal and Friedemann Zenke. The combination of heb- bian and predictive plasticity learns invariant object representations in deep sensory networks. Nature neuroscience, 26(11):1906–1915, 2023. [6] Bernd Illing, Jean Ventura, Guillaume Bellec, and Wulfram Gerstner. Lo- cal plasticity rules can learn deep representations using self-supervised con- trastive predictions, 2021. [7] Diederik P Kingma. Adam: A method for stochastic optimization. arXiv preprint arXiv:1412.6980, 2014. [8] Dorian Krause and Philipp Th¨ornig. Jureca: modular supercomputer at j¨ulich supercomputing centre. Journal of large-scale research facilities JL- SRF, 4:A132–A132, 2018. [9] Ilya Loshchilov and Frank Hutter. Sgdr: Stochastic gradient descent with warm restarts. arXiv preprint arXiv:1608.03983, 2016. [10] R Quian Quiroga, Leila Reddy, Gabriel Kreiman, Christof Koch, and Itzhak Fried. Invariant visual representation by single neurons in the human brain. Nature, 435(7045):1102–1107, 2005. [11] David E Rumelhart, Geoffrey E Hinton, and Ronald J Williams. Learn- ing representations by back-propagating errors. nature, 323(6088):533–536, 1986.

Acknowledgements

We gratefully acknowledge the computing time granted by the JARA Ver- gabegremium and provided on the JARA Partition part of the supercomputer JURECA at Forschungszentrum J¨ulich (Grant no. 30289)

P-031 – Simulation and Data Laboratory Quantum Materials at JSC: Accelerating Quantum Computations on HPC Systems

Edoardo Di Napoli, Forschungszentrum Juelich

Authors: Edoardo Di Napoli, Daniel Rohe, Xinzhe Wu

Institute involved in the work: JSC

Keywords: High performance Computing, Quantum Materials, Numerical Linear Algebra, Research Software Engineering

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

The Simulation and Data Laboratory Quantum Materials at JSC focuses on advancing numerical methods and high-performance computing (HPC) techniques to accelerate quantum materials simulations. Our research spans numerical linear algebra, excitonic Hamiltonian methods, non-equilibrium Green's functions, and tensor network methods, with a strong emphasis on algorithm design, optimization, and scalability.

We specialize in high-performance and parallel matrix computations, developing scalable algebraic eigensolver libraries and tensor computation frameworks. The topical range of our activities spans from non-equilibrium Green's function (NEGF) methods over excitonic methods based on the Bethe-Salpeter equation to density functional theory and applications of funtional renormalisation group methods to correlated electron systems.

Our HPC and parallel computing efforts include performance analysis of large-scale simulations, software modernization, distributed GPU computing, and workflow automation using JUBE and AiiDA. We contribute to community-driven software development and best practices for exploiting multi-GPU architectures, ensuring sustainable and efficient HPC solutions.

We actively lead and participate in major HPC projects, including EoCoE-III, HANAMI, ExaNLA, and large-scale computational initiatives on FUGAKU and EuroHPC systems. Our collaborations extend to the ChASE library for large-scale eigenproblems, functional renormalization group methods, and exascale-ready numerical linear algebra developments.

Key software contributions include ChASE (Chebyshev Accelerated Subspace Eigensolver), ELSI (Electronic Structure Infrastructure), libNEGF (Quantum Transport), and SMG2S (Scalable Matrix Generator). These tools are instrumental in advancing the field of quantum materials research through cutting-edge HPC methodologies.

By integrating advanced numerical algorithms with scalable HPC solutions, we drive the next generation of quantum materials simulations towards exascale computing.

P-032 – The Helmholtz Knowledge Graph: driving the transition towards a FAIR data ecosystem in the Helmholtz Association

Fiona D'Mello, Forschungszentrum Jülich

Authors: Fiona D'Mello, Gabriel Preuß, Jens Bröder, Lucas Kulla, Mustafa Soylu, Said Fathalla, Stefan Sandfeld, Volker Hofmann

Institute involved in the work: IAS-9 , Helmholtz Zentrum Berlin für Materialien und Energie, Berlin, Germany. Deutsches Krebsforschungszentrum, Heidelberg, Germany

Keywords: Metadata, Research Data Infrastructure, Knowledge Graph, FAIR

Research in the Helmholtz Association is carried out in inter- and multidisciplinary collaborations that span between its 18 independently operating research centers across Germany. However, research data and digital assets is heterogeneous in terms of formats, used schemas, record consistency and hosting location. This impairs convergence in a FAIR Helmholtz Data Space.

The Helmholtz Metadata Collaboration (HMC) is taking on this challenge by developing the Helmholtz Knowledge Graph (Helmholtz KG) [1] as a lightweight interoperability layer and semantic harmonization target, that connects Metadata Helmholtz digital assets, which are stored in a decentralized manner. With the KG, we envision (1) providing better cross-organizational access to Helmholtz's (meta)data and information assets on an upper semantic level, (2) harmonizing and optimizing the related metadata across the association, and (3) forming a basis from which the semantic quality and the depths of metadata descriptions is improved and extended into domain and application levels. With recent works [2] we have improved the maturity level of the software to be scaled as more and more data providers are connected and the Graph keeps growing. At the same time we are developing an internal data model with mappings that will allow to aggregate and harmonize data delivered in a from that is consistent with a defined set of semantic standards (Schema.org, DataCite, Dcat, DC). With our effort we want to establish active exchange over which common standards for Helmholtz data providers can emerge and support metadata harmonization.

References

[1] Broeder, J.; Preuss, G.; D'Mello, F.; Fathalla, S.; Hofmann, V.; Sandfeld, S. (2024) The Helmholtz Knowledge Graph: driving the Transition towards a FAIR Data Ecosystem in the Helmholtz Association; The Semantic Web: ESWC 2024, Springer Computer Science Proceedings. doi:10.34734/FZJ-2024-03156 [2] https://codebase.helmholtz.cloud/hmc/hmc-public/unhide

Acknowledgements

This work was supported by (1) the Helmholtz Metadata Collaboration (HMC), an incubator-platform of the Helmholtz Association within the framework of the Information and Data Science strategic initiative

P-033 – So Crazy It Might Just Work: MADRNA

Anton Dorn, JSC

Authors: Anton Dorn, Emile de Bruyn, Fabrice von der Lehr, Alexander Schug, Philipp Knechtges, Stefan Kesselheim

Institute involved in the work: JSC , DLR Cologne

Keywords: Machine Learning, Graph Neural Network, RNA, MD Simulation, Coarse Graining

In Protein structure prediction there have been massive improvements recently with the help of machine learning. In RNA structure prediction however the situation is less ideal due too much sparser experimental data. In principle, molecular dynamics (MD) can provide access to structural dynamics, but the relevant time scales are often out of reach due to prohibitive computational expenses.

A promising approach to scale MD to larger molecules and time scales is machine learning (ML)-based coarse graining. It combines (i) systematic coarse graining, where the degrees of freedom (DOFs) of a molecular system are systematically reduced, and (ii) ML potentials that model the interaction of the new coarse- grained degrees of freedom.

Our approach is based on variational force matching, i.e., we generate trajectories of RNA using classical all-atom simulations, project them down to a coarse-grained level, and train a ML potential to minimize the discrepancy between predicted forces and the forces obtained in simulations. Due to crucial stabilizing effects such as base pairing and stacking, special care is needed when specifying the coarse graining. Our ML potential is built upon the graph neural network SchNet, which enables learning the many-body interactions that govern RNA dynamics.

Preliminary results on a set of tetraloops indicate that our method is able to capture the behavior of RNA correctly. At the same time, it reduces the number of simulated atoms by 2 orders of magnitude and allows for a step size twice as large during simulation, compared to the all-atom setting.

References

[1]: John Jumper et al. Highly accurate protein structure prediction with AlphaFold. Nature 596, 583–589 (2021). DOI: 10.1038/s41586-021-03819-2 [2]: Josh Abramson et al. Accurate structure prediction of biomolecular interactions with AlphaFold 3. Nature 630, 493–500 (2024). DOI: 10.1038/s41586-024-07487-w [3]: Cecilia Clementi et al. Navigating protein landscapes with a machine-learned transferable coarse-grained model. 2023. DOI: 10.21203/rs.3.rs-3578805/v1 [4]: Tristan Cragnolini et al. Coarse-Grained HiRE-RNA Model for Ab Initio RNA Folding Beyond Simple Molecules, Including Noncanonical and Multiple Base Pairings. Journal of Chemical Theory and Computation 11.7 (2015), pp. 3510–3522. DOI: 10.1021/acs.jctc.5b00200 [5]: Kristof T. Schütt et al. SchNet – A deep learning architecture for molecules and materials. The Journal of Chemical Physics 148.24 (2018). DOI: 10.1063/1.5019779 [6]: Brooke E. Husic et al. Coarse Graining Molecular Dynamics With Graph Neural Networks. The Journal of Chemical Physics 153.19 (2020). DOI: 10.1063/5.0026133

P-034 – RNA fitness prediction with sparse physics based models - A way to explore the sequence space

Christian Faber

Authors: Christian Faber, Alexander Schug, Francesco Calvanese, Martin Weigt

Institute involved in the work: JSC

Keywords: RNA, Statistical Physics, Function Prediction

The field of medicine uses macromolecules as a means of therapeutic intervention. Consequently, the functional attributes of these novel molecules are assuming greater significance. To complement the extensive wet-lab experiments, we have devised a series of statistical physics based models that are capable of predicting the fitness of RNA molecules based on one- and two-point mutation scans. The experimental data were employed as training data to fit models of increasing complexity, commencing with an additive model and concluding with a model that accounts for global and local epistasis. The trained models were validated using fitness data from scans with more than two point mutations of the wild-type. In contrast to conventional AI algorithms, the parameters of our models were designed to facilitate direct interpretation. In examining more distant sequences, we can distinguish the corresponding RNA family from random sequences with a high degree of accuracy. Moreover, the models facilitate direct interpretations of evolutionary processes and the significance of epistatic terms. Our model can be used to create a fitness landscape far beyond the experimentally sampled sequence space, thus identifying promising RNA molecules. Furthermore, the extension to the entire sequence space can be used as a blueprint for other molecules, providing a novel avenue for questions in biomolecular design.

P-035 – Performance Evaluation of Vertex-Centric and Algebraic Graph Processing Approaches for BFS and SSSP Using the gem5 Simulator

Carlos Falquez

Authors: Carlos Falquez, Dirk Pleiter, Estela Suarez, Nam Ho

Institute involved in the work: JSC

Keywords: HPC, Architectural simulation, Performance analysis, Graph algorithms, gem5

Graph algorithms are fundamental to a wide range of scientific computing applications, including computational chemistry, machine learning, bioinformatics, social network analysis, and route planning.

State-of-the-art graph processing frameworks typically follow one of two paradigms: vertex-centric or algebraic. Vertex-centric implementations represent graphs as collections of vertices and edges, and traverse the graph by advancing vertex frontiers over connecting edges. This approach results in irregular, data-dependent memory access patterns. Algebraic implementations represent graphs using adjacency matrices and perform graph traversal through iterative sparse matrix-vector multiplications (SpMV) over various algebraic semirings, with memory locality determined by the sparse matrix format used.

In this work, we compare both approaches by benchmarking different implementations of two fundamental graph algorithms: Breadth-First Search (BFS) and Single-Source Shortest Path (SSSP). The vertex- centric implementations are based on Ligra, a state-of-the-art shared-memory graph processing framework. The algebraic implementations utilize a vectorized SpMV kernel based on the SELL-C-σ sparse matrix format.

We evaluate both approaches with respect to runtime, CPU resource utilization, memory access patterns, and scalability on simulated ARM- based architectures using the gem5 computer architecture simulator, which provides detailed performance statistics across a variety of architectural configurations.

Our results show the distinct trade-offs between the two paradigms and provide guidance for selecting the most performant implementation based on algorithm characteristics and target hardware architecture.

P-036 – Semantic description and integration of Helmholtz digital assets using the Helmholtz Digitization Ontology

Said Fathalla

Authors: Said Fathalla, Volker Hofmann, Stefan Sandfeld, Thomas Jejkal

Institute involved in the work: IAS-9 , Karlsruhe Institute of Technology (KIT)

Keywords: Ontology, Digitization, FAIR, interoperability

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

The Helmholtz Association generates vast amounts of digital research data across multiple scientific domains. However, the lack of standardized semantics and interoperable metadata creates heterogeneity that complicates semantic integration and automated processing of these assets. To address and overcome these barriers and to ensure interoperability of the various systems across the Helmholtz Association, we developed the Helmholtz Digitization Ontology (HDO) [1], a mid-level ontology that contains concepts and relationships representing digital assets and processes that appear in the Helmholtz digital ecosystem. The main goal for developing HDO is to serve as a harmonized and machine-actionable institutional reference to represent digital assets and procedures pertinent to their handling and maintenance within Helmholtz.

After the 1st release in late 2024, HDO was adopted and adapted in use cases bridging the Helmholtz research fields. The latest HDO release [2] includes an extension that introduces classes and properties required to semantically represent FAIR Digital Objects (FDOs) based on the Helmholtz Kernel Information Profile (KIP). This representation provides a foundational semantic framework for FDOs being integrated with semantic web technology such as the Helmholtz Knowledge Graph. With this, we ensure the interoperability of systems in the Helmholtz FAIR data space and the machine-actionability of digital assets within it. A comprehensive HTML documentation of HDO is available online [3].

References

[1] https://purls.helmholtz-metadaten.de/hob/hdo.owl
[2] https://codebase.helmholtz.cloud/hmc/hmc-public/hob/hdo
[3] https://purls.helmholtz-metadaten.de/hob/HDO_00000000

P-037 – Active membrane deformations of a synthetic cell-mimicking system

Dmitry Fedosov, Institute of Biological Information Processing, Forschungszentrum Juelich

Authors: Alfredo Sciortino, Andreas Bausch, Gerhard Gompper, Dmitry Fedosov

Institute involved in the work: IAS-2

Keywords: active vesicle, membrane deformation, microtubule network, growing filaments, dynamic triangulation membrane model

POF Topic: P2T4: Molecular and Cellular Information Processing

Biological cells are fascinating micromachines capable of adapting their shape due to the complex interaction between a deformable membrane and the dynamic activity of the cytoskeleton. We investigate the behavior of an active synthetic cell-mimicking system using simulations and experiments [1]. In simulations, the model consists of a fluid vesicle with a few encapsulated growing filaments. In experiments, giant vesicles contain an active cytoskeletal network composed of microtubules, crosslinkers, and molecular motors. These active vesicles show strong shape fluctuations reminiscent of shape changes of biological cells. We analyze membrane fluctuations and show how the intricate coupling between soft confinement and internal active forces results in fluctuation spectra with distinct spatial and temporal scales, differing significantly from those of passive vesicles. Simulations demonstrate the universality of this behavior, quantifying the impact of correlated activity on the dynamics of membrane deformations. This model makes a step toward quantitative description of shape-morphing artificial and living systems.

References

[1] A. Sciortino, H. A. Faizi, D. A. Fedosov, L. Frechette, P. Vlahovska, G. Gompper and A. R. Bausch, Nature Physics, 2025, DOI: 10.1038/s41567-025-02839-3

P-038 – Response functions in residual networks as a measure for signal propagation

Kirsten Fischer

Authors: David Dahmen, Kirsten Fischer, Moritz Helias

Institute involved in the work: IAS-6

Keywords: signal propagation; residual networks; field theory; finite-size effects

Residual networks (ResNets) demonstrate superior trainability and performance compared to feed-forward networks, particularly at greater depths, due to the introduction of skip connections that enhance signal propagation to deeper layers. Prior studies have shown that incorporating a scaling parameter into the residual branch can further improve generalization performance. However, the underlying mechanisms behind these effects and their robustness across network hyperparameters remain unclear.

For feed-forward networks, finite-size theories have proven valuable in understanding signal propagation and optimizing hyperparameters. Extending this approach to ResNets, we develop a finite-size field theory to systematically analyze signal propagation and its dependence on the residual branch's scaling parameter. Through this framework, we derive analytical expressions for the response function, which measures the network's sensitivity to varying inputs. We obtain a formula for the optimal scaling parameter, revealing that it depends minimally on other hyperparameters, such as weight variance, thereby explaining its universality across hyperparameter configurations.

P-039 – Analysis of Glauber Dynamics on Constraint Satisfaction Problems

Niklas Foos, RWTH Aachen / IAS-6 FZJ

Authors: Bastian Epping, Jannik Grundler, Niklas Foos, Alexandru Ciobanu, David Dahmen, Michael Krämer, Moritz Helias

Institute involved in the work: IAS-6

Keywords: Constraint Satisfaction Problems, Optimization, Statistical Physics, Spin Systems, Glauber Dynamics

POF Topic: P2T3: Neuromorphic Computing and Network Dynamics

Constraint Satisfaction Problems (CSPs) are at the heart of complexity theory and relevant in everyday life. Older studies use Hopfield networks to find approximate solutions while recently modern machine learning techniques like graph neural networks became popular for this task. In this study, we use the known mapping of MAX-2-SAT, being a class of CSPs, to a spin glass system from statistical physics and use Glauber dynamics to approximately find its ground state corresponding to the optimal solution of the underlying problem. The Glauber dynamics outperform the traditional Hopfield network approach and can compete with state of the art solvers. Systematic theoretical analysis reveals a spin-dependent effective temperature which for a significant part of spins is non-zero even at temperature T=0. Spins with non-zero effective temperature form a subspace in which the Glauber dynamics continuously flip spins to find better solutions. This is possible despite having no thermal fluctuations since the energy is degenerate so that flips of spins in this free spin space do not require energy. From our theoretical analysis we obtain new solvers which also reach state of the art performance.

P-040 – Bridging Scales in Computational Neuroscience: A Deep Learning Approach to Parameter Mapping from Spiking Networks to Brain Oscillations

Sinovia Fotiadou

Authors: Sinovia Fotiadou

Institute involved in the work: JSC

Keywords: NEST, TVB, AI, HPC

This study, conducted within the Virtual Brain Twin Project (VBT), presents a computational framework that bridges mesoscopic spiking neural network dynamics and macroscopic brain oscillations using high- performance computing (HPC). Large-scale neuronal simulations in NEST generate vast amounts of spike time data, which are converted into neuronal firing rates that capture cellular-level activity. These firing rates serve as inputs to a deep learning pipeline composed of two sequential models. First, a transformer-based neural network predicts key parameters (conduction speed, coupling strength, and global delay) for neural mass models in The Virtual Brain (TVB). Second, a surrogate multilayer perceptron (MLP) approximates the output of TVB simulations, specifically of the two-state Reduced Wong- Wang model, which then generates macroscopic oscillatory signals.

Central to this approach is a bridging loss that compares the macroscopic firing rates produced by the surrogate MLP with the original mesoscopic firing rates from NEST. The resulting error is backpropagated to refine the transformer's parameter predictions. Rigorous hyperparameter optimization via Optuna and 5-fold cross- validation ensures robust generalization. Successful minimization of this loss validates that estimating the parameter manifolds between spiking neural networks and neural mass models via computational scaling using AI is feasible, thereby confirming the proof-of-concept and demonstrating the transformative potential of HPC, NEST, and TVB in neuroscience.

Acknowledgements

Supervised by Dr. Sandra Diaz

P-041 – Why community matters more than ever - collaborative community engagement, training and education in large research projects and infrastructures

Maren Frings

Authors: Maren Frings, Boris Orth, Sandra Diaz

Institute involved in the work: JSC

Keywords: Key strategies for Collaborative Community Engagement, Networking, Training and Education, Transfer of Results, Sustainability

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

Building a research community is a strategic necessity, not an option. Fostering greater engagement and strong collaborative networking can create sustainable flows and promote the long-term growth of communities and associated research infrastructures. Complemented by community-specific education and training programmes, the transfer of knowledge, skills and research results for the benefit of the community is sustainably promoted. Based on more than 10 years of experience in working with large research projects and accompanying communities with divers scientific backgrounds we, the Simulation and Data Lab Neuroscience present key strategies and best practices based on our experience with the neuroscience community on how to bring the right people together and how to create spaces, where audiences don’t just listen and consume content but engage with it, discuss it, and contribute to the further development of the research project and infrastructure.

P-042 – A new staggered action in Lattice QCD

Davide Giusti, Forschungszentrum Jülich

Authors: Davide Giusti

Institute involved in the work: JSC

Keywords: Lattice QCD

Many theory predictions in particle physics are limited by our ability to quantify hadronic effects and the main goal of large-scale simulations using the lattice formulation of QCD is the evaluation of the nonperturbative QCD effects in physical processes. In this contribution we present our progress in exploring the scaling properties of a new, improved lattice formulation of the QCD action with staggered fermions, called 4HEX, promising reduced discretization errors and better control of the continuum limit. To this end we have generated a number of dedicated lattice gauge ensembles which will be used for various frontier scientific investigations in particle physics, such as spectroscopy, weak decays and structure of hadrons, and the calculation of the muon g-2.

P-043 – Supercomputing in a Browser - Easy access to WebTools for increased Productivity

Jens Henrik Goebbert, Forschungszentrum Jülich, Jülich Supercomputing Centre *and*

Tim Kreuzer, Forschungszentrum Juelich GmbH, Juelich Supercomputing Centre

Authors: Jens Henrik Goebbert, Tim Kreuzer

Institute involved in the work: JSC

Keywords: WebTools, Data Analysis, Productivity, Supercomputing, Cloud

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

Jupyter-JSC at https://jupyter.jsc.fz-juelich.de makes “Supercomputing in the Browser” since 7 years now as easy as it sounds for everyone with access to the large supercomputers at Jülich Supercomputing Centre and for any Helmholtz employee provides those tools on the cloud.

Interactive exploration and analysis of large amounts of data from scientific simulations, in-situ visualization and application control are convincing scenarios for explorative sciences. Based on the open source software JupyterLab, a way has been available for some time now that combines interactive with reproducible computing while at the same time meeting the challenges of support for the wide range of different software workflows. Even on supercomputers, the method enables the creation of documents that combine live code with narrative text, mathematical equations, visualizations, interactive controls, and other extensive output.

The service continously develops further to a general WebApp portal and providing tools like RStudio, VSCode, remote desktop, and growing. For experts Binder-functionality and general container-support ensures that it can be fully customized using resources of the JSC-Cloud.

On project-specific URLs with project-specific branding and -functions Jupyter-JSC is used as the collaboration platform by a number of projects (InHPC Portal Gauss Centre, Jupyter4NFDI, JUNIQ, CoE Raise, CoE Combustion, EuroCC-GCS). Its comprehensive functionality is being further developed and used across multiple centers.

P-044 – Climate Science - Simulation and Data Laboratory

Sabine Griessbach

Authors: Sabine Griessbach, Amirhossein Nikfal, Catrin Meyer, Farah Khosrawi, Lars Hoffmann, Ling Zou, Nils Nobre Wittwer, Olaf Stein, Sergey Sukov, Yen-Sen Lu, Yiran Zhang

Institute involved in the work: JSC

Keywords: Climate Science, Atmosphere, HPC

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

The Simulation and Data Laboratory (SDL) Climate Science links Earth system modeling research with HPC by helping the scientific community to efficiently deploy comprehensive coupled Earth system models on the latest computing architectures. Our work focuses on the optimization of Earth system models for performance and scalability, and the portability of these models to new hardware architectures of modular supercomputing systems. Along with simulations, data play an important role. The establishment of efficient workflows and the handling of large data sets are inseparably linked to the achievement of performance enhancements in Earth system modelling. Therefore, the Jülich MeteoCloud was created and is a well-received resource. At the same time, the SDL conducts its own research. Our research focuses on atmospheric transport, gravity waves, remote sensing, clouds and aerosols, and atmospheric chemistry. Model-data fusion plays a prominent role in our research and showcases the capabilities of JSC's HPC systems in terms of data and computing resources. Our own code developments are the Massive-Parallel Trajectory Calculations (MPTRAC), a tool for simulating the Lagrangian transport of air parcels and analyzing large atmospheric datasets, and the JUelich RApid Spectral SImulation Code (JURASSIC), a fast infrared radiative transfer model for analyzing atmospheric remote sensing measurements. Both codes are freely available to the community. The SDL Climate Science participates in the Helmholtz Joint Labs and collaborates with the Institute of Climate and Energy Systems Troposphere (ICE-3) and Stratosphere (ICE-4) in the CASA SDL Climate Science for atmospheric and climate simulations on exascale supercomputers.

P-045 – Hardware Sovereignty and Efficiency – Unlocking Innovation with Hardware-Software Co-Design

Kaveh Haghighi Mood, Jülich Supercomputing Centre *and*

Stepan Nassyr, Jülich Supercomputing Centre

Authors: Kaveh Haghighi Mood, Stepan Nassyr, Jayesh Badwaik, Nam Ho, Andreas Herten

Institute involved in the work: JSC

Keywords: HPC, AI, RISC-V, ARM, Hardware-Software Co-design

JSC plays a key role in advancing Europe's autonomous HPC/AI ecosystem through its contributions to major EuroHPC JU projects, including EPI, EUPILOT, and DARE. These initiatives aim to develop energy-efficient, European-designed processors that reduce reliance on external technologies by leveraging hardware-software co-design and modern instruction set architectures such as ARM and RISC-V. This poster demonstrates key aspects of these projects, highlighting JSC's contributions to achieving technological sovereignty in Europe's HPC/AI landscape.

P-046 – Deep learning with layer-local objectives

Damir Iagudin, Forschungszentrum Jülich

Authors: Damir Iagudin, Viet Anh Khoa Tran, Willem Wybo

Institute involved in the work: PGI-15

Keywords: Layer-local learning, Vision Transformers, Adapters, Self-supervised learning, Proto-tasks, DINO, Task modulation, Representation learning, Parameter-efficient tuning, Hierarchical representations

End-to-end backpropagation dominates deep learning, yet exploring alternative training paradigms like layer-local learning is crucial for understanding representation formation. This work investigates training deep networks, specifically Vision Transformers (ViTs), using layer-local objectives. We propose a two-stage approach: first, self- supervised pre-training of the backbone network using DINO pipeline; second, freezing the backbone and training lightweight IA3 adapters inserted into hidden layers using various supervised “proto-tasks” (e.g., object/scene classification, depth estimation, jigsaw puzzles). These task objectives are applied locally at different network depths, modulating representations without end-to-end gradient flow through the entire network. Our experiments reveal that optimal performance for different tasks often peaks at specific intermediate layers, suggesting a hierarchical task representation. Furthermore, task modulation via adapters proved essential for convergence and performance, particularly when training objectives target non-final layers. These findings demonstrate the potential of combining self- supervised pre-training with layer-local, task-modulated supervised tuning to develop performant deep networks capable of generating robust and versatile features, offering a path towards potentially more interpretable and efficient learning.

P-047 – Sensory and behavioural tuning along the dorsal pathway

Junji Ito, INM-10

Authors: Junji Ito, Simon Essink, Alexa Riehle, Thomas Brochier, Sonja Gruen

Institute involved in the work: IAS-6

Keywords: Neuroscience, spike train analysis, generalized linear model, dorsal visual pathway, motor

POF Topic: P2T3: Neuromorphic Computing and Network Dynamics

Directional tuning of motor cortex neurons is typically characterized by a sinusoidal tuning curve with a preferred direction (PD) represented by its peak. While PDs across neurons were assumed to be uniformly distributed, recent experiments reported a bimodal distribution of hand movement PDs when the movements are constrained to a horizontal plane. Several modelling studies attribute this to the limb biomechanics, which indicates more kinetic (muscle force based) rather than kinematic (movement parameter based) representation in the motor cortex. We conducted neuronal recordings in behaving macaques to elucidate to what extent this kinetic tuning extends down along the dorsal pathway. The monkeys were trained for a visually guided reaching task in the horizontal plane. Spiking activity was recorded in visual (V1/V2), parietal (DP, 7A) and motor (M1/PMd) areas. To estimate the tuning curve of each neuron to sensory and behavioural modalities, we regressed the spiking activity of each neuron on all available behavioural and sensory covariates (visual input, eye/hand position, saccade, hand movement direction and speed) at once by using generalized linear models. The model fitting results reveal a gradual shift in visual and motor tuning along the dorsal pathway: increasing of motor and decreasing of visual tuning towards the motor cortex. We confirm the bimodal hand movement PD distribution in M1/PMd, and also find, after eliminating the confounding effect of the visual tuning, similar bimodal PD distributions in V1/V2, DP and 7A, suggesting an influence of limb biomechanics even in the lower hierarchy levels of the dorsal visual stream.

P-048 – Cognitive flocks: order-disorder transitions and threat evasion

Priyanka Iyer, IBI-5

Authors: Priyanka Iyer, Cecilia Soroco, Gerhard Gompper

Institute involved in the work: IAS-2

Keywords: Active Matter, Collective Behaviour

POF Topic: P2T4: Molecular and Cellular Information Processing

Directed self-propulsion is ubiquitous in living organisms. Ranging from E.Coli dispersing in biofilms to migrating bird flocks, living organisms are constantly out-of equilibrium. By sensing their environment and adjusting their movement, organisms can exhibit emergent patterns and collective behaviors, such as self-organization in human crowds [1], bird flocks, and fish schools. The Inertial Spin Model (ISM) was introduced to explain the fast and robust propagation of information in bird flocks [2], when only alignment interactions are considered. However, more generally, agents exhibit a variety of interactions like local avoidance, cohesion and threat evasion. We show how such behaviors can be incorporated within the framework of the ISM. It is found that local avoidance introduces emergent noise in the system, triggering an order-disorder transition. Exploring the flock dynamics near this transition reveals a complex interplay between cohesion, alignment, and local avoidance, resulting in diverse behaviors such as pronounced shape and density fluctuations, and diffusive motion of the flock. Lastly, by applying the model to a stationary threat scenario, we analyze flock properties that govern threat information propagation in the flock.

References

[1] Iyer, P. et al. , Comm. Phys. 7.1 (2024): 379. [2] Attanasi, A. et al. , Nat. Phys. 10, 691-696, (2014)

P-049 – Solving Rayleigh-Bénard Convection with Fourier Neural Operator

Chelsea Maria John, Juelich Supercomputing Center

Authors: Chelsea Maria John, Andreas Herten, Stefan Kesselheim, Daniel Ruprecht

Institute involved in the work: JSC , Technical University of Hamburg

Keywords: FNO , CFD

Rayleigh-Bénard convection, is a classic fluid dynamics problem, with applications in geophysical, astrophysical, and industrial flows. Fourier Neural Operator (FNO) leverages neural networks and Fourier analysis to efficiently model spatiotemporal dynamics in fluid systems, offering a promising avenue for accurate and scalable simulations. In this poster, results on the application of FNO for tackling the 2-D Rayleigh-Benard convection equations is presented.

P-050 – A Versatile Exascale-Ready Fast Multipole Method

Ivo Kabadshow, Juelich Supercomputing Centre

Authors: Ivo Kabadshow, Holger Dachsel, Arijus Lengvenis, Ioannis Lilikakis

Institute involved in the work: JSC

Keywords: FMM, HPC, GPU, Linear Coulomb Solver, MD

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

The most costly part of molecular simulations is the computation of pairwise electrostatic long-range interactions. Thus, the efficiency of calculating these interactions is decisive for the whole simulation.

Therefore, techniques like the particle-mesh Ewald method (PME) were adopted. Such O(N log N) methods excel for homogeneous particle distributions in MD, but lack performance for sparse particle distributions. Additionally, the scaling to a large number of cores is severely limited due to global communication requirements.

To resolve both problems the Fast Multipole Method (FMM) can be utilized.

On this poster, we present a versatile, linear scaling FMM for MD simulations. We describe capabilities (mixed periodic boundary conditions, arbitrary accuracy), as well as features like error control and automatic runtime minimization of this numerical method. Beside domain science considerations, we will also showcase the challenges arising from mapping such an algorithm to modern hierarchical and heterogeneous Exascale hardware.

P-051 – Learnable polynomial, trigonometric, and tropical activations

Ismail Khalfaoui, Forschungszentrum Jülich

Authors: Ismail Khalfaoui, Stefan Kesselheim

Institute involved in the work: JSC

Keywords: Deep Learning, Learnable activations, Orthogonal function bases, Tropical polynomials, Polynomial mapping, Deep neural networks, ImageNet-1K, OpenWebText, Transformers, GPT2, Convolutional networks, ConvNeXt, Initialization scheme, PyTorch

This work investigates scalable neural networks with learnable activation functions based on orthogonal function bases and tropical polynomials, targeting ImageNet-1K classification and next token prediction on OpenWebText. Traditional activations, such as ReLU, are static. In contrast, learnable activations enable the network to adapt dynamically during training. However, stability issues, such as vanishing or exploding gradients, arise with improper variance management in deeper networks. To remedy this, we propose an initialization scheme that single-handedly preserves unitary variance in transformers and convolutional networks, ensuring stable gradient flow even in deep architectures. Extensive experiments demonstrate that networks with Hermite, Fourier, and Tropical-based learnable activations significantly improve over GPT-2 and ConvNeXt networks in terms of accuracy and perplexity in train and test, highlighting the viability of learnable activations in large-scale tasks. The activation functions developed here are the subject of a library coded entirely in pure PyTorch: torchortho, available at: https://github.com/K-H-Ismail/torchortho.

P-052 – Inference of network structures in a Bayesian setting

Matthias Klaus

Authors: David Dahmen, Matthias Klaus, Moritz Helias

Institute involved in the work: IAS-6

Keywords: Bayesian inference, subsampling, Dynamic mean field theory, Gaussian process, recurrent neural network, disorder average, student-teacher model

Inference of model parameters from heavily subsampled data is a challenge in all sciences. In neuroscience in particular, today's recording techniques allow one to access finite time windows of a few hundred to thousands of neurons. Since they are embedded in strongly connected networks of 10^5 neurons, the recorded data will be considerably influenced by the structure of these unobserved parts. Theoretical descriptions of the problem often assume spatial and temporal homogeneity across the system, i.e. that structure and activity of the entire network, on a statistical level, is close to the recorded part.

Here we model this statistical homogeneity by the connectivity variance and the variance of a globally independent driving white noise. Estimates for these parameters exist from prior experiments. Consequently, we use a Bayesian approach to obtain a local connectivity posterior, provided locally recorded activity. The theory involves a marginalization over unobserved activity, which is exact for a linear network whose activity is a Gaussian process. This condition can be relaxed by reasonably assuming a large network and applying dynamic mean field theory [1] [2]. We find that reconstruction of local connectivity is possible if the influence from unobserved parts reduces to a colored noise whose statistics is estimated correctly. On the other hand, the mean-field assumptions (infinite network, diminishing connectivity) require a careful interpretation of results and limit the possibility of statements about the unobserved network.

References

[1] Sompolinsky, Crisanti, Sommers 1988 [2] Schuecker, Goedeke, Helias 2018

P-053 – DevOps and Science Support for Brain Research: A Multidisciplinary Approach for High-Performance Computing and Infrastructure Integration

Wouter Klijn, Forschungszentrum Jülich GmbH, Institute for Advanced Simulation, Jülich Supercomputing Centre (JSC), Simulation and Data Lab Neuroscience, JARA, 52425 Jülich | Germany

Authors: Wouter Klijn, Ekaterina Zossimova, Jithu Murugan, Krishna Singh, Lena Oden, Marissa Diaz Pier, Sandra Diaz

Institute involved in the work: JSC

Keywords: computational neuroscience; brain research; EBRAINS research infrastructure; co-design

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

We present a multidisciplinary approach to advance neuroscience research, combining scientific consultancy, DevOps, and High- Performance Computing (HPC). Our method has successfully supported diverse projects, from 2D brain slice data analysis to digital twinning solutions.

Our process translates scientific requirements into technical specifications, guided by monthly co-design meetings addressing ethics, GDPR, HPC, and education. Behind the scenes, DevOps manages virtualization, complex ecosystem development, and HPC integration, exemplified by EUROHPC platform containerization.

Our approach facilitates efficient neuroscience research, contributing to the EBRAINS infrastructure and related projects. We demonstrate this through four key processes:

1. **Use-Case Analysis and Formalization:** We systematically analyze and formalize neuroscience use-cases, converting complex scientific needs into clear, feasible technical specifications.
2. **Integration of Large Use-Case Toolboxes:** We integrate diverse, large-scale tools using DevOps, ensuring portability, scalability, and efficiency. An example is the Virtual Brain Twin (VBT) project's tool integration for clinical applications.
3. **Deployment and Application of Integrated Environments:** We deploy and apply integrated environments for benchmarking system performance and implementing energy-efficient practices, reducing energy consumption while maintaining high performance.
4. **Additional Considerations:** We address crucial aspects through monthly co-design meetings, including ethics, GDPR compliance, HPC resource allocation, and education, ensuring proactive challenge resolution and informed decision-making.

Acknowledgements

Co-funded by the European Union (Grant No. HORIZON-INFRA-2022-SERV-B-01, EBRAINS 2.0 project).

P-054 – Facilitating provenance tracking in NEST simulations with Alpaca

Cristiano A. Köhler, Institute for Advanced Simulation (IAS-6), Jülich Research Centre, Jülich, Germany; RWTH Aachen University, Aachen, Germany

Authors: Cristiano A. Köhler, Moritz Kern, Sonja Grün, Michael Denker

Institute involved in the work: IAS-6

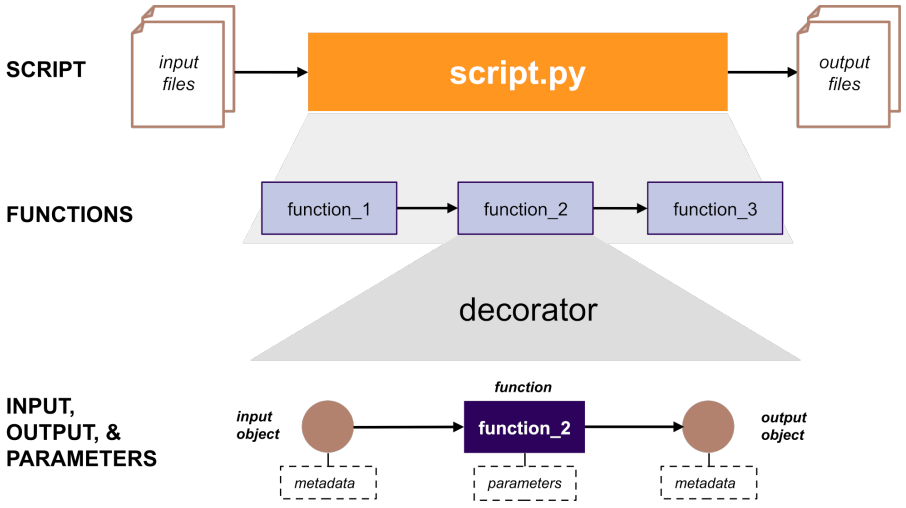
Keywords: neural simulation, data analysis, provenance, FAIR, Python

POF Topic: P2T3: Neuromorphic Computing and Network Dynamics

Neural simulations using NEST are typically executed by a Python script that configures the simulator, builds the network, and runs the simulation. The output files can be further analyzed to understand the neural activity. To interpret the findings, the simulation setup, network connectivity, and parameters of the neuronal and synaptic models need to be known. However, obtaining this information usually requires referring to the original script, making sharing results in collaborative settings challenging. Furthermore, simulation parameters may change over time, and tracking those changes is difficult among collaborators with access to shared output files. Therefore, the results of a NEST simulation lack detailed provenance to link each output to the description of how the network was instantiated and run.

We developed Alpaca (RRID:SCR_023739) [1] to capture provenance when executing Python scripts. Alpaca records function execution details and data objects using decorators (see Figure). Here, we demonstrate how Alpaca tracks provenance in NEST simulations and subsequent analyses with Elephant (RRID:SCR_003833) [2]. First, we show how it captures end-to-end provenance in workflows running multiple NEST simulations with distinct parameters. Second, we illustrate how data objects are annotated with simulation details using the Neo library [3] to identify the data source in the simulation. Third, we detail how network creation using PyNEST is linked to each data output and analysis result.

This approach improves the representation of simulated data and analysis results according to the FAIR principles [4]: provenance enhances findability, a standardized data model supports interoperability, and detailed descriptions facilitate data reuse.



References

[1] Köhler, C.A., Ulianych, D., Grün, S., Decker, S., Denker, M., 2024. Facilitating the sharing of electrophysiology data analysis results through in-depth provenance capture. eNeuro 11, ENEURO.0476-23.2024. https://doi.org/10.1523/ENEURO.0476-23.2024

[2] Denker, M., Yegenoglu, A., Grün, S., 2018. Collaborative HPC-enabled workflows on the HBP Collaboratory using the Elephant framework. Neuroinformatics 2018, P19. https://doi.org/10.12751/incf.ni2018.0019

[3] Garcia, S., Guarino, D., Jaillet, F., Jennings, T., Pröpper, R., Rautenberg, P.L., Rodgers, C.C., Sobolev, A., Wachtler, T., Yger, P., Davison, A.P., 2014. Neo: an object model for handling electrophysiology data in multiple formats. Frontiers in Neuroinformatics 8, 10. https://doi.org/10.3389/fninf.2014.00010

[4] Wilkinson, M.D., Dumontier, M., Aalbersberg, Ij.J., Appleton, G., Axton, M., Baak, A., Blomberg, N. et al., 2016. The FAIR Guiding Principles for scientific data management and stewardship. Scientific Data 3, 160018. https://doi.org/10.1038/sdata.2016.18

Acknowledgements

This work is performed as part of the HDS-LEE and receives funding from the Helmholtz Association of German Research Centres, EU Grants 785907 (HBP), 945539 (HBP), and 101147319 (EBRAINS 2.0), the Joint Lab “Supercomputing and Modeling for the Human Brain”, and the NRW network iBehave (NW21-049).

P-055 – Application of ML to the Characterization of Grain- and Phase Boundaries by EBSD

Peter J. Konijnenberg, FZ Juelich IAS-9

Authors: Peter J. Konijnenberg, Stefan Sandfeld, Stefan Zaefferer

Institute involved in the work: IAS-9 , Max Planck Institute for Sustainable Materials

Keywords: EBSD, ML, Grain Boundary, Anti-Phase Boundary, Point-group

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

Over the last decade significant advancements were reported in Electron Backscatter Diffraction (EBSD) via the use of pattern matching algorithms that essentially use the full information content by cross-correlating the acquired patterns with a forward-simulation, [1,2]. Apart from some early attempts [3], the application of neural networks to the entire pattern analysis process was reported only relatively recently, [4,5]. Here forward-simulated patterns are utilized to train a convolutional neural network (CNN), which then can be used for the task of analyzing acquired patterns. We report about the development and application of such an approach to the analysis of grain and phase boundaries.

In the vicinity of grain boundaries, depending on the grain boundary inclination w.r.t. the electron beam, frequently a superposition of two Kikuchi patterns of both adjacent grains is observed. In the case of Hough-based analysis, the presence of overlapping Kikuchi patterns often results in a zone of mis- or non-indexed map points along grain boundaries. We demonstrate and evaluate how the ML-method deals with these overlapping patterns.

In polar materials, anti-phase boundaries (APBs) separate domains of opposing chemical ordering. Due to Friedel's rule, classical EBSD techniques are bound to fail on these boundaries. Hence, only the orientation of the overarching Laue group can be determined. As was shown by Winkelmann et al. [6], a point-group correct orientation analysis can overcome this through the additional use of pattern matching with dynamically simulated patterns. We demonstrate that the ML-based method is able to achieve this in a single analysis step.

References

1 Chen, Y. H., et al. Microscopy and Microanalysis 21.3 (2015): 739-752. 2 Hielscher, R. et al. Ultramicroscopy 207 (2019): 112836. 3 Schwarzer, R.A., and Sukkau, J. Advanced Engineering Materials 5.8 (2003): 601-606. 4 Dipendra, J. et al. Microscopy and Microanalysis 24.5 (2018): 497-502. 5 Ding, Z. et al. Acta Materialia 199 (2020): 370-382 6 Winkelmann, A. and Nolze, G. Applied Physics Letters 106.7 (2015).

P-056 – Event-driven eligibility propagation: combining efficiency with biological realism

Agnes Korcsak-Gorzo, Institute for Advanced Simulation (IAS-6), Computational and Systems Neuroscience, Forschungszentrum Jülich, Jülich, Germany; Fakultät 1, RWTH Aachen University, Aachen, Germany

Authors: Agnes Korcsak-Gorzo, Jesús A. Espinoza Valverde, Jonas Stapmanns, Hans Ekkehard Plesser, David Dahmen, Matthias Bolten, Sacha J. van Albada, Markus Diesmann

Institute involved in the work: IAS-6

Keywords: spiking neural networks, synaptic plasticity, machine learning, neural computation

POF Topic: P2T3: Neuromorphic Computing and Network Dynamics

Neural networks have permeated our lives through the advancement of AI algorithms. While they offer powerful solutions across various applications, their biological roots also provide a window into understanding human learning. This has led to growing interest in finding biological analogies within successful machine learning techniques, resulting in numerous biologically inspired learning rules.

The brain performs complex tasks with remarkable energy efficiency. Mimicking these mechanisms could unlock scalable, energy-efficient learning algorithms - crucial as AI's energy demands grow. This work develops a scalable biologically inspired learning algorithm that remains computationally efficient, and performs well by exploiting biological principles such as sparsity.

We build on e-prop [1], a learning algorithm for spiking recurrent neural networks that approximates backpropagation through time [2]. We port it from TensorFlow [3] to the NEST simulator [4], designed for large-scale spiking neural networks. We convert its time-driven weight updates into an event-driven scheme, minimizing redundant computations, enhance the model with biologically grounded features, and validate it on the neuromorphic MNIST dataset [5]. Our implementation maintains learning performance and efficiency, scaling to millions of neurons on the CPU partition of the JURECA supercomputer.

Many AI frameworks, like TensorFlow or PyTorch [6], rely on time- driven updates. Our method provides a blueprint for translating these - especially biologically inspired rules - into more efficient event- driven schemes. At the intersection of physics, AI, simulation technology, and neuroscience, this work shows how nature can inspire computationally efficient algorithms. Its scalability supports simulations of behavioral tasks, enabling deeper insights into learning mechanisms.

References

[1] Bellec, G., Scherr, F., Subramoney, A., Hajek, E., Salaj, D., Legenstein, R., & Maass, W. (2020). A solution to the learning dilemma for recurrent networks of spiking neurons. Nature Communications, 11 (1), 3625. https://doi.org/10.1038/s41467-020-17236-y

[2] Werbos, P. J. (1990). Backpropagation through time: what it does and how to do it. Proceedings of the IEEE, 78 (10), 1550–1560. https://doi.org/10.1109/5.58337

[3] Abadi, M., Agarwal, A., Barham, P., Brevdo, E., Chen, Z., Citro, C., Corrado, G. S., Davis, A., Dean, J., Devin, M., Ghemawat, S., Goodfellow, I., Harp, A., Irving, G., Isard, M., Jia, Y., Jozefowicz, R., Kaiser, L., Kudlur, M., ... Zheng, X. (2016). TensorFlow: Large-scale Machine Learning on Heterogeneous Distributed Systems. arXiv. https://doi.org/10.48550/arXiv.1603.04467

[4] Espinoza Valverde, J. A., Müller, E., Haug, N., Schöfmann, C. M., Linssen, C., Senk, J., Spreizer, S., Trensch, T., Lober, M., Jiang, H., Kurth, A., Acimovic, J., Korcsak-Gorzo, A., Welle Skaar, J.-E., Terhorst, D., Stapmanns, J., Graber, S., de Schepper, R., Eppler, J. M., ... Plesser, H. E. (2024, May). Nest 3.7. https://doi.org/10.5281/zenodo.10834751

[5] Orchard, G., Jayawant, A., Cohen, G. K., & Thakor, N. (2015). Converting static image datasets to spiking neuromorphic datasets using saccades. Frontiers in Neuroscience, 9, 437. https://doi.org/10.3389/fnins.2015.00437

[6] Ansel, J., Yang, E., He, H., Gimelshein, N., Jain, A., Voznesensky, M., Bao, B., Bell, P., Berard, D., Burovski, E., Chauhan, G., Chourdia, A., Constable, W., Desmaison, A., DeVito, Z., Ellison, E., Feng, W., Gong, J., Gschwind, M., ...

Chintala, S. (2024). PyTorch 2: Faster Machine Learning Through Dynamic Python Bytecode Transformation and Graph Compilation. 29th ACM International Conference on Architectural Support for Programming Languages and Operating Systems, Volume 2 (ASPLOS '24). https://doi.org/10.1145/3620665.3640366

Acknowledgements

This work was supported by Joint Lab SMBH; HiRSE_PS; NeuroSys (Clusters4Future, BMBF, 03ZU1106CB); EU Horizon 2020 Framework Programme for Research and Innovation (945539, Human Brain Project SGA3) and Europe Programme (101147319, EBRAINS 2.0); computing time on JURECA (JINB33) via JARA Vergabegremium at FZJ; and Käte Hamburger Kolleg: Cultures of Research (c:o/re), RWTH Aachen (BMBF, 01UK2104).

P-057 – Ab-initio investigation of transition metal-superconductor interfaces

Adamantia Kosma, Forschungszentrum Juelich

Authors: Adamantia Kosma, Philipp Ruessmann, Stefan Bluegel

Institute involved in the work: PGI-1

Keywords: ab-initio simulations, KKR method, superconductivity

The realisation of Majorana-based topologically protected qubits requires a careful design and optimization of material interfaces for superconductor (SC) / topological insulator (TI) heterostructures. To this end, we perform ab-initio simulations to investigate the superconducting properties at the interface of transition metal overlayers (M = Os, Ir, Pt, Au) deposited on a Nb(110) film. Our simulations are performed using the open-source JuKKR code [1], which allows us to study real materials. The density functional theory calculations are based on the full-potential Korringa-Kohn-Rostoker (KKR) Green function method for determining the electronic structure of materials, and its Kohn-Sham Bogoliubov-de Gennes (KS-BdG) extension [1, 2] for studying superconducting properties. In our study we explore the possibility to control the work function mismatch through the overlayer, which is essential to overcome spurious band bending effect at typical SC/TI interfaces. Furthermore, we uncover the proximity induced superconductivity in the metal overlayers and discuss related details in their electronic structure. Our findings show that some of these structures might be promising material candidates for interfacing a TI with a superconductor without unwanted band bending effects at SC/M/TI interfaces.

References

[1] JuDFTteam/JuKKR (2022). doi: 10.5281/zenodo.7284738 [2] P. Rüßmann, and S. Blügel, Phys. Rev. B 105, 125143 (2022). [3] Jülich Supercomputing Centre, Journal of large-scale research facilities 7, A182 (2021).

P-058 – AI in the Simulation and Data Lab Neuroscience

Kai Krajsek, Forschungszentrum Jülich GmbH

Authors: Kai Krajsek, Claudia Comito, Hanno Scharr

Institute involved in the work: JSC , IAS-8

Keywords: High-Performance Computing, Deep Learning, Neuroscience

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

The Simulation and Data Lab (SDL) Neuroscience integrates neuroscience with High-Performance Computing (HPC) and provides extensive support tailored to the specific needs of the neuroscience community. This poster presents the AI activities of SDL Neuroscience using dedicated examples from the perspective of infrastructure support, method development, and research. Neuroscience has scaled up its analysis of brain imaging data, making HPC resources needed. We present a polarised light imaging pipeline for high throughput of data on the JSC HPC systems in collaboration with neuroscientists from INM-1. Deep learning (DL) methods have overtaken the analysis of neuroimaging data, as have many other research areas. One component of the success of DL is the availability of reliable software libraries like PyTorch and TensorFlow. Unfortunately, these DL libraries have not been developed with HPC in mind, and HPC features are still being integrated. We describe concepts that allows automatic differentiation as well as effective tensor computation across different computing nodes, which is only partially possible with current libraries. As an example of AI research, we present a learning scheme developed in collaboration with IAS-8 that preserves symmetries in the data, achieving state-of-the-art performance for training computer vision foundation models.

P-059 – Dynamical mean-field theory of critical slowing down in high-dimensional regression problems

Jakob Kramp

Authors: Jakob Kramp, Javed Lindner, Moritz Helias

Institute involved in the work: IAS-6

Keywords: machine learning, kernel regression, dynamical mean-field theory, disorder average

Despite significant recent progress, the analytical understanding of machine learning remains limited. Networks in the highly- overparametrized regime are well described by linear regression in feature space, also known as kernel regression. This view enables analytical insights into complex behaviors, such as the double descent phenomenon [Belkin19] or spectral bias [Canatar21]. In this work, we investigate the effects of data disorder on the learning dynamics of kernel ridge regression. Unlike static approaches for computing disorder-averaged weight statistics, we employ a dynamic method yielding a moment generating functional from the stochastic equation of motion. This enables the analysis of both the stationary distribution of the trained weights and the learning dynamics. Within this framework, we use a dynamic mean-field approximation to derive self-consistency equations for the response function and the autocorrelation of the network parameters. We identify a disorder- dependent critical point in the response function, derive a fluctuation-dissipation theorem, and confirm our theoretical results through numerical experiments below the critical point. The work provides a stepping stone to predict the training dynamics in deep networks.

References

Belkin, Mikhail et al. (2019). “Reconciling modern machine-learning practice and the classical bias–variance trade-off”. In: Proceedings of the National Academy of Sciences 116.32, pp. 15849–15854.

Canatar, Abdulkadir et al. (2021). “Spectral bias and task-model alignment explain generalization in kernel regression and infinitely wide neural networks”. In: Nature Communications 12.1, p. 2914.

P-060 – Cognitive maps in brains and machines

Sven Krausse, PGI-15, Forschungszentrum Jülich *and*

Alpha Renner, Forschungszentrum Jülich

Authors: Sven Krausse, Emre Neftci, Friedrich T. Sommer, Alpha Renner

Institute involved in the work: PGI-15 , Redwood Center for Theoretical Neuroscience, UC Berkeley

Keywords: Neuromorphic Computing, Computational Neuroscience, Cognitive maps

POF Topic: P2T3: Neuromorphic Computing and Network Dynamics

While we observe our world sequentially, our brains consolidate this information into cognitive maps linking allocentric positions with semantic information[1]. These maps form for physical space and abstract concept spaces, enabling efficient storage, inference, and generalization.

The allocentric code needed to form cognitive maps is generated in the entorhinal hippocampal formation through place[2] and grid cells[3]. Additionally, head direction cells[4] provide a sense of orientation. Both allocentric position and head direction use movement integration and anchoring through visual cues. However, how these modalities can be integrated in one system remains an open question.

In our project, we study the formation of allocentric spatial codes from sequential, egocentric observations. Based on the continuous attractor model[5], we provide a mathematical framework[6] to describe grid cell activity and link it to hyperdimensional computing[7], enabling the integration of movement and visual cues. Additionally, we analyzed experimental data of head direction cells in mice[8] to identify the anchoring mechanisms of these cells. Surprisingly, we found parallax effects in the head direction system, indicating a simple cue anchoring mechanism in the orientation system[9].

In our ongoing work, we combine the findings of head direction and grid cell models to build a visually guided path integration model that continuously integrates its angular and translatory movements while using visual cues, producing a robust spatial representation.

In the future, we plan to introduce learning mechanisms to link this spatial code with observed semantic information and use these cognitive maps for goal-directed navigation and sequence learning tasks.

References

[1]: Buzsaki and Moser - "Memory, navigation and theta rhythm in the hippocampal-entorhinal system" (Nature Neuroscience) [2]: O'Keefe and Dostrovsky 1971 - "The hippocampus as a spatial map. Preliminary evidence from unit activity in the freely-moving rat" (Brain Research) [3]: Hafting et al. 2005 - "Microstructure of a spatial map in the entorhinal cortex" (Nature) [4]: Taube et al. 1990 - "Head-direction cells recorded from the postsubiculum in freely moving rats" (The Journal of Neuroscience) [5]: McNaughton 2006 - "Path integration and the neural basis of the 'cognitive map'" (Nature reviews Neuroscience) [6]: Krausse et al. 2025 - "A grid cell-inspired structured Vector algebra for cognitive maps" (ArXiv, accepted at NICE 2025 conference) [7]: Plate 1995 - "Holographic reduced representations" (IEEE Trans. Neural Networks) [8]: Duszkiewicz et al. 2020 - "Local origin of excitatory–inhibitory tuning equivalence in a cortical network" (Nature Neuroscience) [9]: Krausse et al. 2025 - "Head-Direction Cells in Postsubiculum Show Systematic Parallax Errors During Visual Anchoring" (under review)

Acknowledgements

This research is funded by VolkswagenStiftung [CLAM 9C854].

P-061 – Computing the Band Gap for the Metallization Transition of Hydrogen using Variational Quantum Monte Carlo

Edgar Landinez Borda, FJZ-IAS/JSC

Authors: Edgar Landinez Borda, Claudia Filippi, Markus Holzmann, Saverio Moroni

Institute involved in the work: JSC

Keywords: High Pressure Physics, Ab initio, Electronic Structure, Quantum Monte Carlo

POF Topic: P2T1: Quantum Materials

Understanding the high-pressure metallization of hydrogen remains a central challenge in condensed matter physics. Here, we present a periodic variational quantum Monte Carlo (VMC) approach, adapting multistate optimization—originally developed for finite systems—to directly compute the band gap at different pressures from path integral Monte Carlo (PIMC) configurations. Utilizing a CIS-type trial wave function, our results for the band gap at high pressures are consistent with previous QMC calculations based on quasiparticle gaps and show good agreement with GW. This work provides a compelling characterization of the electronic transition in hydrogen, highlighting the power of our adapted QMC methodology for studying periodic systems under extreme conditions.

P-062 – Feature learning in deep neural networks close to criticality

Javed Lindner, Forschungzentrum Jülich

Authors: Javed Lindner, Kirsten Fischer, David Dahmen, Zohar Ringel, Michael Krämer, Moritz Helias

Institute involved in the work: IAS-6

Keywords: Field Theory, Neural Networks, Feature Learning, Kernels

Neural networks excel due to their ability to learn features, yet its theoretical understanding continues to be a field of ongoing research. We develop a finite-width theory for deep non-linear networks, showing that their Bayesian prior is a superposition of Gaussian processes with kernel variances inversely proportional to the network width. In the proportional limit where both network width and training samples scale as $N,P \to \infty$ with P/N fixed, we derive forward-backward equations for the maximum a posteriori kernels, demonstrating how layer representations align with targets across network layers. A field-theoretic approach links finite-width corrections of the network kernels to fluctuations of the prior, bridging classical edge-of-chaos theory with feature learning and revealing key interactions between criticality, response, and network scales.

P-063 – Modeling and simulating spiking neurons and synaptic plasticity with NESTML on SpiNNaker

Charl Linssen, Simulation Lab Neuroscience, Forschungszentrum Jülich GmbH

Authors: Charl Linssen, Pooja Babu, Levin Schmidt, Bernhard Rumpe, Abigail Morrison

Institute involved in the work: JSC

Keywords: modeling, dynamical system, neuromorphic, simulation, neuron, synapse, plasticity

NESTML is a domain-specific modeling language for spiking neuronal networks incorporating synaptic plasticity [1]. NESTML features a concise yet expressive syntax, inspired by Python. It supports researchers in computational neuroscience by making models easier to write and maintain, and to make models more findable, accessible, interoperable and reusable ('FAIR' principles). Models can be used in dynamical simulations of spiking neural networks at very large scale (with millions of neurons and synapses), by means of high performance simulation code generated by the NESTML toolchain. The code extends a simulation platform (such as NEST Simulator [3] or SpiNNaker [4]) with new and easy to specify neuron and synapse models, formulated in NESTML. Combining a user-friendly modeling language with automated code generation makes large-scale neural network simulation accessible to neuroscience researchers without requiring any training in computer science [2].

Models specified in the NESTML syntax are processed by an open-source toolchain that generates fast code for a given target simulator platform. It was originally developed for NEST Simulator [3]; here we extend it with support for the SpiNNaker neuromorphic hardware platform [4]. We demonstrate our approach with code generation for a balanced random network of integrate-and-fire neurons with postsynaptic currents in the form of decaying exponential kernels. The dynamics of the network are solved using exact integration [5]. We validate the results by means of comparison of statistical properties of the network dynamics against those obtained from the NEST Simulator running on a standard CPU as a reference.

References

[1] https://github.com/nest/nestml/ [2] Blundell et al., Frontiers in Neuroinformatics 12, 2018 [3] Gewaltig & Diesmann, Scholarpedia 2(4), 2007 [4] Furber et al., Proceedings of the IEEE 102(5), 2014 [5] Rotter and Diesmann, Biological Cybernetics 81, 1999

P-064 – Learning sequence timing and control of recall speed in networks of spiking neurons

Melissa Lober

Authors: Melissa Lober, Markus Diesmann, Tom Tetzlaff, Younes Bouhadjar

Institute involved in the work: IAS-6

Keywords: Sequence learning, spiking neuronal network, time representation

Processing sequential inputs is a fundamental aspect of brain function, underlying tasks such as sensory perception, reading, and mathematical reasoning. Sequence processing involves learning the order and timing of elements, predicting future events, detecting unexpected deviations, and recalling learned sequences. The Spiking Temporal Memory (STM) model [1], a biologically inspired spiking neuronal network, provides a framework for key aspects of sequence processing. In its original version, however, it can not learn the timing of sequence elements. Further, it remains an open question how the speed of sequential recall can be flexibly modulated. We propose a mechanism in which the duration of sequence elements is represented by repeated activations of element specific neuronal populations. The STM model can thereby represent even long time intervals, providing a biologically plausible basis for learning and recalling not only the order of sequence elements, but also complex rhythms. Additionally, we demonstrate that oscillatory background inputs can serve as a clock signal and thereby provide a robust mechanism for controlling the speed of sequence recall. Modulation of oscillation frequency and amplitude enable a stable recall across a wide range of speeds, offering a biologically relevant strategy for flexible temporal adaptation. Our findings suggest that time is encoded by unique and sparse spatio- temporal patterns of neural activity, and that the speed of sequence recall is correlated to the characteristics of global oscillatory activity, observed in EEG or LFP recordings. In summary, our results contribute to the understanding of sequence processing and time representation in the brain.

References

[1] Bouhadjar, Y., Wouters, D. J., Diesmann, M., Tetzlaff, T. (2022), Sequence learning, prediction, and replay in networks of spiking neurons, PLOS Computational Biology 18(6):e1010233

P-065 – Hadron physics with the Jülich-Bonn model: determining the light baryon resonance spectrum

Christian Schneider *and*

Deborah Ronchen *and*

Oleh Luniachek

Authors: Deborah Ronchen, Christian Schneider, Oleh Luniachek

Institute involved in the work: IAS-4

Keywords: Hadron physics

The goal of this longtime project is to determine the spectrum of light baryon resonances, which encodes the key to understand the strong force at medium energies. The extraction of the spectrum from experimental data is challenging and sophisticated dynamical coupled-channel approaches, such as the Jülich-Bonn model, are the method of choice. They are, however, numerically costly, which necessitates the use of HPC systems. Among other challenges, a systematic quantification of uncertainties is so far not possible. The main objective in the coming years is therefore the transition to a Bayesian parameter estimation using the Hamiltonian Monte Carlo (HMC) algorithm, allowing for a determination of resonance parameter uncertainties in a statistically well-defined way.

P-066 – Memory in Neural Networks

Rishabh Mallik, Forschungszentrum Juelich

Authors: Rishabh Mallik, Younes Bouhadjar

Institute involved in the work: Other , PGI-14

Keywords: Memory Augmented networks, Sequence modelling, AI, Meta-learning, formal languages, chomsky hierarchy

Memory is very essential for sequential tasks with long contexts. It requires storing information from the entire seen context in a memory to be able to carry out further processing. Different deep learning architectures maintain memory internally, like RNNs and Transformers, whereas some architectures have an explicit memory like memory augmented neural networks - MANNs (eg Neural Turing Machines[[1]][1]).

To formally test how good these networks use their memory, we construct toy tasks from the Chomsky hierarchy, which gives a hierarchy of formal languages depending on if they can be detected/generated using algorithms with or without an external memory, and how flexibly can these algorithms access this memory.

We pick tasks like parity, ignore, association etc, with real-world applications, and see if MANNs still hold up against other modern sequence modelling networks[[2]][2]. We test memory networks with memory updates done by the network itself vs memory updates done by gradient descent as in Titans[[3]][3] and Neural Memory Networks[[4]][4], checking if gradient updated memories generalize better on these tasks.

We explore possibility of using MANNs for Meta-learning [[5]][5]. Goal of Meta learning is to make the model adapt to new data without much tuning. Tuning requires many gradient steps and could result in catastrophic forgetting. MANNs offer ability to quickly encode and retrieve new information, hence potentially adapt to new tasks without the problems with gradient methods. We do experiments to compare their adaptability over world model learning tasks.

[1]: https://arxiv.org/abs/1410.5401
[2]: https://arxiv.org/abs/2207.02098
[3]: https://arxiv.org/abs/2501.00663
[4]: https://arxiv.org/abs/1907.09720
[5]: https://arxiv.org/abs/1605.06065

References

[1] Graves, A., Wayne, G., & Danihelka, I. (2014c, October 20). Neural turing machines. arXiv.org. https://arxiv.org/abs/1410.5401 [2] Delétang, G., Ruoss, A., Grau-Moya, J., Genewein, T., Wenliang, L. K., Catt, E., Cundy, C., Hutter, M., Legg, S., Veness, J., & Ortega, P. A. (2022b, July 5). Neural networks and the Chomsky hierarchy. arXiv.org. https://arxiv.org/abs/2207.02098 [3] Behrouz, A., Zhong, P., & Mirrokni, V. (2024b, December 31). Titans: Learning to Memorize at Test Time. arXiv.org. https://arxiv.org/abs/2501.00663 [4] Munkhdalai, T., Sordoni, A., Wang, T., & Trischler, A. (2019, July 23). Metalearned neural memory. arXiv.org. https://arxiv.org/abs/1907.09720 [5] Santoro, A., Bartunov, S., Botvinick, M., Wierstra, D., & Lillicrap, T. (2016, May 19). One-shot Learning with Memory-Augmented Neural Networks. arXiv.org. https://arxiv.org/abs/1605.06065

P-067 – SEANERGYS: Software for Efficient and Energy-Aware Supercomputers

Samuel Maloney, Jülich Supercomputing Centre (JSC), Forschungszentrum Jülich (FZJ)

Authors: Samuel Maloney, SEANERGYS Project Members

Institute involved in the work: JSC

Keywords: High performance computing; Energy efficient computing; Monitoring; Data analysis; Artificial intelligence; Dynamic scheduling

POF Topic: P1T2: Supercomputing & Big Data Infrastructures

SEANERGYS creates an integrated European software solution that optimises resource utilisation and reduces the energy used for real- world workload mixes. It therefore improves the throughput of HPC systems, generating more R&D results for a given energy budget. The solution consists of a comprehensive monitoring infrastructure (CMI), an Artificial Intelligence data analytics system (AIDAS), and a dynamic scheduling and resource management system (DSRM).

The CMI gathers data from hardware and software sensors, and correlates it with scheduler information to identify jobs that do not fully utilize allocated resources. Users receive automatic feedback on energy and resource use for each run, plus information on how to optimize these. The AIDAS leverages AI models trained with a vast set of operational data from the participating HPC sites. It fingerprints resource usage patterns, predicts future job behaviour, and identifies complementary job profiles for potential co-scheduling. Finally, the DSRM utilizes these insights to develop scheduling policies that maximize resource utilization and energy efficiency, and supports jobs/applications with dynamic and adaptable resource profiles.

Acknowledgements

The SEANERGYS project has received funding from the European High-Performance Computing Joint Undertaking (JU). The JU receives support from the European Union's Horizon Europe research and innovation programme and Germany, Spain, Italy, France, Greece, Czechia, and Luxembourg.

P-068 – ATML NUMERICAL AND STATISTICAL METHODS

Sina Mattfeldt

Authors: Sina Mattfeldt, Andreas Kleefeld

Institute involved in the work: JSC

Keywords: Partial differential equations, boundary integral equations, boundary element method, non-linear eigenvalue problems, ill-posed inverse problems

The ATML “Numerical and Statistical Methods” is part of the “Mathematics and Education” department of the Jülich Supercomputing Centre. It develops, implements, and tests new procedures/methods in the area of stochastic ordinary and partial differential equations that arise, for example, in image processing, acoustic, electromagnetic, and elastic scattering problems, and reaction- diffusion-advection equations. In this context, the group also deals with algorithms for the solution of ill-posed inverse problems and the computation of eigenvalue problems. The poster presents the topics and current research results of the group.

P-069 – Vortex formation and odd viscosity in a chiral active fluid

Joscha Mecke

Authors: Gerhard Gompper, Joscha Mecke, Marisol Ripoll, Yongxiang Gao

Institute involved in the work: IAS-2

Keywords: chiral active matter; odd viscosity; active turbulence; colloidal rotors

Materials consisting of active particles with an intrinsic rotation can be considered as chiral active matter. We study a colloidal chiral active system, consisting of magnetic microrotors of diameter 0.8 μm in an externally applied rotating magnetic field. The stabilised colloids synchronously rotate with the rotating field and solely interact via steric and hydrodynamic interactions, granting odd and active stresses already at low densities and large colloidal separations. We address the system by means of experiments as well as particle based hydrodynamics simulations (MPC) of the active colloidal suspension. The rotors' transverse, anti-symmetric, and non-reciprocal interactions lead to a pair-rotation about the centre of mass and subsequently to the formation of multiscale vortices. Energy is injected on the particle level and is transported to the largest scales in the system, unless it is dissipated at a hydrodynamic damping length, a process reminiscent of turbulence, even in the absence of dominant inertial contributions. The rich phenomenology of our system additionally includes odd diffusion and enhancement of effective diffusive transport by the introduction of obstruction, directed transport by virtue of symmetry breaking at confining walls, and correlations between vorticity and density which allow for a measurement of the system's odd viscosity.

P-070 – The Future of Climate Modeling - Performance and Possibilities of ICON on Next-Gen Hardware

Catrin I. Meyer

Authors: Andreas Herten, Catrin I. Meyer, Lars Hoffmann, Manoel Römmer, Sabine Griessbach, Yen-Sen Lu

Institute involved in the work: JSC

Keywords: Climate Modeling, ICON, high resolution, exascale-ready, JEDI, JUWELS Booster

The ICOsahedral Non-hydrostatic (ICON) model is a modelling framework for weather, climate, and environmental prediction that used for operational weather forecasting by the German and Swiss Weather Service. It is also an Earth System Model for climate simulations, featuring a general circulation model of the atmosphere, a land module, and an ocean model. While the atmosphere component has been adapted to run on GPUs, the ocean component still runs on CPUs, requiring a hybrid configuration for coupled simulations. The ICON model is available under an open-source license.

JSC is involved in several projects to implement an ICON based storm and eddy resolving Earth system. The IFCES2 (Optimization of simulation algorithms for exascale supercomputers to compute the Earth system model ICON) project aims to develop new methods for parallel execution of ICON simulation algorithms on heterogeneous and modular exascale systems. The WarmWorld project focuses on redefining the ICON code structure to identify areas for performance improvement and exploring new programming concepts. A rigorous analysis of ICON's performance was conducted on the JUWELS Booster (NVIDIA A100 GPUs) and the Jupiter Exascale Development Instrument (JEDI) demonstrator (NVIDIA GH200 GPUs) as part of JUREAP (JUPITER Research and Early Access Program). In this context, ICON demonstrated effective scaling across the entire JUWELS Booster system and validated the expected performance gains from A100 to GH200 GPUs on JEDI. This demonstrates that ICON is exascale-ready. A tool for continuous integration and continuous deployment, Buildbot, is utilized to provide continously benchmarking of ICON on the JSC systems.

P-071 – High-throughput computing with FLEUR

Gregor Michalicek, FZJ

Authors: Gregor Michalicek, Daniel Wortmann, Jens Bröder, Stefan Blügel

Institute involved in the work: PGI-1

Keywords: FLEUR; AiiDA; Linearized augmented-plane-wave-method; Density functional theory; High-throughput computing; Workflow automatization

Today's condensed matter research demands often imply the need to produce data for large sets of test materials. This need is especially amplified for simulations, be it in the context of materials design or for guiding experiments. A bottleneck when performing many calculations is the degree of manual interaction needed to obtain stable and high-quality results from a complex simulation software. For the all-electron full-potential linearized augmented-plane-wave density functional theory code FLEUR, we developed a fully automatic means for performing large amounts of calculations. This involves the connection of the FLEUR code to the AiiDA automatization framework, as well as the definition of parameter setup profiles for precise and stable calculations. On this poster we sketch the resulting infrastructure and demonstrate its power.

P-072 – Data Science Challenges and Opportunities: Lessons from the Jülich LOFAR Archive

Arpad Miskolczi, Jülich Supercomputing Centre

Authors: Arpad Miskolczi, Cristina Manzano, Holger Stiele

Institute involved in the work: JSC

Keywords: Archives, Big Data, Astronomy

POF Topic: P1T2: Supercomputing & Big Data Infrastructures

The Forschungszentrum Jülich has been hosting the German part of the LOFAR archive since 2013. It is Germany's most extensive radio astronomy archive, currently storing nearly 24 petabytes (PB) of data. Future radio telescopes are expected to require a dramatic increase in long-term data storage.

We have analysed the current data management of the Jülich LOFAR Data Archive, including ingestion, storage system, export to the long-term storage layer, and request chain. We studied data usage over the last 10 years and examined the underlying data access patterns. We also estimated the archive's energy consumption.

From our assessment, we identified hardware-related limiting factors, such as network bandwidth and cache pool availability, as well as software aspects like workflow adjustments and parameter tuning, as the main performance bottlenecks in data storage. We also concluded that the primary challenge in providing data from the archive lies in retrieving and staging data from the tape layer.

Building on this analysis, we suggest ways to mitigate these issues in the future and offer guidelines for successfully addressing the challenges future big data science will bring.

P-073 – Study of Protein Folding and Design using Quantum Annealing

Sandipan Mohanty, Forschungszentrum Jülich GmbH

Authors: Sandipan Mohanty

Institute involved in the work: JSC

Keywords: Quantum Annealer, biophysics, folding, design

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

Using a simple lattice model with a 2 letter amino acid alphabet (H: hydrophobic and P: polar), we have explored the important biophysical problems of protein folding and protein design. Our formulation of these problems features a simple algebraic form for the Hamiltonian irrespective of the system size and composition. Since exact results are available from for lattice HP chains up to a size of 30, we were able to thoroughly validate our approach. The D-Wave advantage quantum annealer successfully identifies the ground state of the HP model protein chain in 100% of cases. For a few longer protein chains with up to 64 amino acids, where exact enumerations were not available but extensive Monte Carlo studies exist, the D-Wave hybrid annealer found the correct ground states within minutes, once again with a 100% success rate. Applying the same technique to the protein design problem, we found novel HP protein sequences with the same ground state as the largest systems we studied for folding. In contrast to the sequences used for folding, some of our newly found sequences had unique rather than degenerate ground states.

References

”Folding lattice proteins with quantum annealing”, Anders Irbäck, Lucas Knuthson, Sandipan Mohanty, and Carsten Peterson, Phys. Rev. Research 4, 043013 (2022)

”Using quantum annealing to design lattice proteins”, Anders Irbäck, Lucas Knuthson, Sandipan Mohanty, and Carsten Perterson, Phys. Rev. Research 6, 013162 (2024)

P-074 – Learning to Learn on Quantum Computing

Hanna Mohr

Authors: Hanna Mohr, Sandra Diaz

Institute involved in the work: JSC

Keywords: HPC, Quantum Computing, Neuroscience

L2L is an open-source tool for hyperparameter optimization for high- performance computing systems. It is based on the concepts of learning to learn and meta-learning. This poster details the use of L2L in conjunction with HPC systems and the JUPSI Quantum Annealer, which is hosted by JSC, as a backend for L2L. The poster further explores the potential of community detection in brain connectomics to support this application.

P-075 – Towards a time-scale specific subspace for brain inter-area communication

Daniel Moreno Soto, Department of Physics, Faculty 1, RWTH Aachen University, Germany. Institute for Advanced Simulation (IAS-6) Jülich Research Centre, Germany.

Authors: Daniel Moreno Soto, David Dahmen, Lars Schutzeichel, Moritz Helias, Simon Musall

Institute involved in the work: IAS-6 , IBI-3

Keywords: inter-area communication, NEST simulator, second criticality, neural networks, communication subspace, between-area communication, neuronal dynamics, linear rate neuron

Brain-wide neural function involves the communication between neural networks from distinct anatomical areas and different evolutionary antiquity, as in the mammal cortico-thalamo-cortical loop formed by S1, M2, and TH [1, 2]. Despite its evident importance, the mechanisms by which the information is relayed in this “inter-area” communication remain hazy. Additionally, it is still unknown how the operation at criticality, a property of neural networks that contributes to their computational capabilities [3-5], integrates into the inter-area picture. Dynamics at criticality can be understood through disordered random networks and entail a wide distribution of correlations and eigenmodes—representing neurons acting in unison—with diverse time scales [6-9]. The orchestrated action of different areas must derive from the evolutionary optimization of networks at criticality in a way that conserves local operation and also allows for efficient inter- area communication. In this work, we explore if the projection neurons between areas belong to a linear subspace of communication composed of modes coupling in a manner that respects the time-scale hierarchy of the local networks. We couple two recurrent networks of linear rate neurons with input noise via the eigenmodes of the connectivity matrices of each network. Preliminary results sending a signal between two real coupled modes show that the transfer function acts as a double low-pass filter with cutoff frequencies depending on the eigenvalues of the modes. Future work will include the connection of an arbitrary number of complex modes and experimental validation of the inter-area connections for the S1-M2-TH loop in mice.

References

[1] Isabelle Ferezou, Florent Haiss, Luc J. Gentet, Rachel Aronoff, Bruno Weber, and Carl C.H. Petersen. Spatiotemporal dynamics of cortical sensorimotor integration in behaving mice. Neuron, 56:907–923, 12 2007.

[2] Zengcai V. Guo, Nuo Li, Daniel Huber, Eran Ophir, Diego Gutnisky, Jonathan T. Ting, Guoping Feng, and Karel Svoboda. Flow of cortical activity underlying a tactile decision in mice. Neuron, 81:179–194, 1 2014.

[3] T. Toyoizumi and L. F. Abbott. Beyond the edge of chaos: Amplification and temporal integration by recurrent networks in the chaotic regime. Physical Review E - Statistical, Nonlinear, and Soft Matter Physics, 84:051908, 11 2011.

[4] Guillermo B. Morales and Miguel A. Muñoz. Optimal input representation in neural systems at the edge of chaos. Biology, 10:702, 8 2021.

[5] Lorenzo Tiberi, Jonas Stapmanns, Tobias Kühn, Thomas Luu, David Dahmen, and Moritz Helias. Gell-mann-low criticality in neural networks. Physical Review Letters, 128:168301, 4 2022.

[6] Carsen Stringer, Marius Pachitariu, Nicholas Steinmetz, Matteo Carandini, and Kenneth D. Harris. High-dimensional geometry of population responses in visual cortex. Nature, 571:361–365, 7 2019.

[7] David Dahmen, Hannah Bos, and Moritz Helias. Correlated fluctuations in strongly coupled binary networks beyond equilibrium. Physical Review X, 6:031024, 8 2016.

[8] Yu Hu and Haim Sompolinsky. The spectrum of covariance matrices of randomly connected recurrent neuronal networks with linear dynamics. PLOS Computational Biology, 18:e1010327, 7 2022.

[9] David Dahmen, Moritz Layer, Lukas Deutz, Paulina Anna Dąbrowska, Nicole Voges, Michael Von Papen, Thomas Brochier, Alexa Riehle, Markus Diesmann, Sonja Grün, and Moritz Helias. Global organization of neuronal activity only requires unstructured local connectivity. ELife, 11, 1 2022.

P-076 – Advancing Numerical Lattice Field Theory Towards the Exascale Regime

Fabian Nieto Castellanos, JSC *and*

Simon Schlepphorst

Authors: Aniket Sen, Bartosz Kostrzewa, Eric Gregory, Fabian Nieto Castellanos, Giovanni Pederiva, Luna Sophie Meyer, Simon Schlepphorst, Stefan Krieg, Travis Whyte

Institute involved in the work: JSC

Keywords: Kokkos, performance portability, Numerical Lattice Field Theory, benchmarking, algorithms

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

The advancement of numerical lattice field theory (LFT) to the exascale regime poses unique challenges due to the scaling of algorithms to a very large number of nodes as well as the rapidly changing hardware landscape. The algorithms underlying numerical LFT must therefore be scalable and performance-portable. We report on the status of the B02 and B06 projects under CRC 1639 NumeriQs, which aim to develop scalable multilevel algorithms and performance-portable software to run efficiently on heterogeneous High-Performance Computing systems based on the Modular Supercomputing Architecture (MSA). The performance of the multilevel methods under development in B06 are demonstrated against classical methods and benchmarks of the performance-portable software in development under B02 are presented.

P-077 – Climate data services in JSC

Amirhossein Nikfal, Forschungszentrum Jülich

Authors: Amirhossein Nikfal, Olaf Stein

Institute involved in the work: JSC

Keywords: Datalad, JSC Cloud, THREDDS, Climate Data

POF Topic: P1T2: Supercomputing & Big Data Infrastructures

In this project, we have utilized a combination of high-performance computing (HPC) and cloud-based services to efficiently manage, process, and distribute climate data. On the HPC system, we employed DataLad for version-controlled data management, which can be seamlessly installed by using EasyBuild, enabling robust and scalable workflows for handling large volumes of climate model outputs. Additionally, we integrated cloud services, notably the THREDDS Data Server on the JSC Cloud platform, to provide standardized, web- accessible distribution of NetCDF datasets, facilitating seamless data sharing and interoperability within the scientific community. This hybrid approach enhances both the reproducibility and accessibility of climate data workflows, aligning with best practices in open science and data stewardship.

P-078 – Time-to-first-spike encoding in layered networks evokes label-specific synfire chain activity

Jonas Oberste-Frielinghaus, Institute for Neuroscience and Medicine INM-6 and INM-10 and Institute for Advanced Simulation (IAS-6) Research Center Juelich, Juelich, Germany Theoretical Systems Neurobiology, Faculty I, RWTH Aachen, Germany

Authors: Jonas Oberste-Frielinghaus, Anno Kurth, Julian Göltz, Laura Kriener, Junji Ito, Mihai Petrovici, Sonja Gruen

Institute involved in the work: IAS-6

Keywords: information coding, synchronization and oscillation, system dynamics, neural computation

POF Topic: P2T3: Neuromorphic Computing and Network Dynamics

While artificial neural networks (ANNs) have achieved remarkable success in various tasks, they lack two major characteristic features of biological neural networks: spiking activity and operation in continuous time. This makes it difficult to leverage knowledge about ANNs to gain insights into the computational principles of the real brains. However, training methods for spiking neural networks (SNNs) have recently been developed to create functional SNN [3]. In this study we analyze the structure and activity of a multilayer feedforward SNN trained to classify MNIST.

In response to a sample, the input layer generates a volley of spikes, identified as a pulse packet (PP) [2], propagating through the hidden layers. In deeper layers, spikes in a PP get more synchronized and the neurons providing spikes to the PP become more specific to the sample label, leading to a characteristic sparse representation of the sample label in deep layers. Analysis of connection weights reveals that a correct classification is achieved by propagating spikes through a specific pathway across layers, composed of neurons with strong excitatory effects on the correct output neuron.

The revealed connectivity structure and the propagation of spikes as a PP agree with the notion of the synfire chain (SFC) [1]. In our network, multiple parallel SFCs natually emerge through the training, representing each input label by activation of one particular SFC. This leads to sparser encoding of the input label in deeper layers, and increased the linear separability of layer-wise activity.

References

[1] Abeles, M. (1982). Local Cortical Cuircits. Springer; Abeles, M. (1991). Corticonics: Neural Circuits of the Cerebral Cortex. Cambrige University Press [2] Diesmann, M. et al. (1999). Stable propagation of synchronous spiking in cortical networks. Nature, 402(6761), 529-533. doi:10.1038/990101 [3] Göltz, J. et al. (2021). Fast and energy-efficient neuromorphic deep learning with first-spike times. Nature Machine Intelligence, 3(9), 823-835. doi:10.1038/s42256-021-00388-x

P-079 – Multi-scale Spiking Network Model of Human Cerebral Cortex

Renan Oliveira Shimoura, Institute for Advanced Simulation (IAS-6), Jülich Research Centre, Jülich, Germany

Authors: Jari Pronold, Alexander van Meegen, Renan Oliveira Shimoura, Hannah Vollenbröker, Mario Senden, Claus C. Hilgetag, Rembrandt Bakker, Sacha van Albada

Institute involved in the work: IAS-6

Keywords: connectivity, large-scale, neural network, resting-state activity, simulation

Data-driven models at cellular resolution exist for various brain regions, yet few for human cortex. We present a comprehensive point- neuron network model of a human cortical hemisphere that integrates diverse experimental data into a unified framework bridging cellular and network scales [1]. Like a previous large-scale spiking model of macaque cortex [2,3], our work investigates how resting-state activity emerges in cortical networks.

The model represents one hemisphere via the Desikan-Killiany parcellation (34 areas), with each area implemented as a 1 mm² microcircuit that distinguishes cortical layers. It aggregates multimodal data, including electron microscopy for synapse density, cytoarchitecture from the von Economo atlas [4], DTI-based connectivity [5], and local connection probabilities from the Potjans- Diesmann microcircuit [6]. Human neuron morphologies [7] guide layer- specific inter-area connectivity. The full-density model, comprising 3.47 million leaky integrate-and-fire neurons and 42.8 billion synapses, was simulated using NEST on the JURECA-DC supercomputer.

Simulations show that equal strength for local and inter-area synapses yields asynchronous irregular activity that deviates from experimental observations. When inter-area connections are strengthened relative to local synapses, both microscopic spiking statistics from human medial frontal cortex and macroscopic resting-state fMRI correlations are reproduced [8]. In the latter scenario, consistent with empirical findings during visual imagery [9], sustained activity flows primarily from parietal through occipital and temporal to frontal areas.

This open-source model enables systematic exploration of structure- dynamics relationships. Future work may leverage the Julich-Brain Atlas to refine the parcellation and incorporate detailed cytoarchitectural and receptor data [10]. The model code is available at https://github.com/INM-6/human-multi-area-model.

References

[1] Pronold, J., van Meegen, A., Shimoura, R. O., Vollenbröker, H., Senden, M., Hilgetag, C. C., Bakker, R., & van Albada, S. J. (2024). Multi-scale spiking network model of human cerebral cortex. Cerebral Cortex, 34(10). https://doi.org/10.1093/CERCOR/BHAE409. [2] Schmidt, M., Bakker, R., Hilgetag, C. C., Diesmann, M., & van Albada, S. J. (2018). Multi-scale account of the network structure of macaque visual cortex. Brain Structure and Function, 223(3), 1409–1435. https://doi.org/10.1007/s00429-017-1554-4. [3] Schmidt, M., Bakker, R., Shen, K., Bezgin, G., Diesmann, M., & van Albada, S. J. (2018). A multi-scale layer-resolved spiking network model of resting-state dynamics in macaque visual cortical areas. PLOS Computational Biology, 14(10), e1006359. https://doi.org/10.1371/journal.pcbi.1006359. [4] Von, Economo C (2009). Cellular structure of the human cerebral cortex. Karger Medical and Scientific Publishers. Triarhou. Basel, CH. https://doi.org/10.1159/isbn.978-3-8055-9062-4. [5] van Essen, D. C., Smith, S. M., Barch, D. M., Behrens, T. E. J., Yacoub, E., & Ugurbil, K. (2013). The WU-Minn Human Connectome Project: An overview. NeuroImage, 80, 62–79. https://doi.org/10.1016/J.NEUROIMAGE.2013.05.041. [6] Potjans, T. C., & Diesmann, M. (2014). The Cell-Type Specific Cortical Microcircuit: Relating Structure and Activity in a Full-Scale Spiking Network Model. Cerebral Cortex, 24(3), 785–806. https://doi.org/10.1093/cercor/bhs358. [7] Mohan, H., et al. (2015). Dendritic and Axonal Architecture of Individual Pyramidal Neurons across Layers of Adult Human Neocortex. Cerebral Cortex, 25(12), 4839–4853. https://doi.org/10.1093/CERCOR/BHV188. [8] Minxha, J., Adolphs, R., Fusi, S., Mamelak, A. N., & Rutishauser, U. (2020). Flexible recruitment of memory-based choice representations by the human medial frontal cortex. Science (New York, N.Y.), 368(6498). https://doi.org/10.1126/science.aba3313. [9] Dentico, D. et al. (2014). Reversal of cortical information flow during visual imagery as compared to visual perception. NeuroImage, 100, 237–243. https://doi.org/10.1016/J.NEUROIMAGE.2014.05.081. [10] Zilles, K., & Palomero-Gallagher, N. (2017).

Multiple transmitter receptors in regions and layers of the human cerebral cortex. Frontiers in Neuroanatomy, 11, 78. https://doi.org/10.3389/fnana.2017.00078.

Acknowledgements

This work was supported by the German Research Foundation (DFG) Priority Program "Computational Connectomics" (SPP 2041; Project 347572269), the EU Grant 945539 (HBP), EBRAINS 2.0 Project (101147319), the Joint lab SMHB, and HiRSE_PS. The use of the JURECA-DC supercomputer in Jülich was made possible through VSR computation grant JINB33. Open access publication funded by DGF Grant 491111487.

P-080 – EBRAINS Germany

Boris Orth, Forschungszentrum Jülich, JSC

Authors: Boris Orth, Maren Frings, Sandra Diaz

Institute involved in the work: JSC , IAS-6, INM-9

Keywords: EBRAINS, Human Brain Project, HBP, ESFRI, EDIC, digital research infrastructure, neuroscience, brain research

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

EBRAINS is a unique digital research infrastructure (RI) for neuroscience, brain medicine and brain-inspired technologies, created by the European Human Brain Project (HBP). It is part of the 2021 roadmap of ESFRI (European Strategy Forum on Research Infrastructures). Organised around a central coordinating hub in Brussels, Belgium, the EBRAINS RI provides data, tools and services for collaborative brain and brain-related research to the community through a pan-European network of National Nodes. EBRAINS Germany, the German National Node of EBRAINS, was officially established by a cooperation agreement in 2023 and currently consists of nine member institutions, led by Forschungszentrum Jülich and coordinated by a team based at JSC. A major goal of EBRAINS Germany and the national nodes in general is to secure political support and sustainable funding at the national level, to make EBRAINS a permanent RI and to enable its transition towards a European Digital Infrastructure Consortium (EDIC). The poster will present the current status of EBRAINS Germany, including an overview of the services and tools already provided or planned for the future, its organisational structure, as well as recent and planned activities.

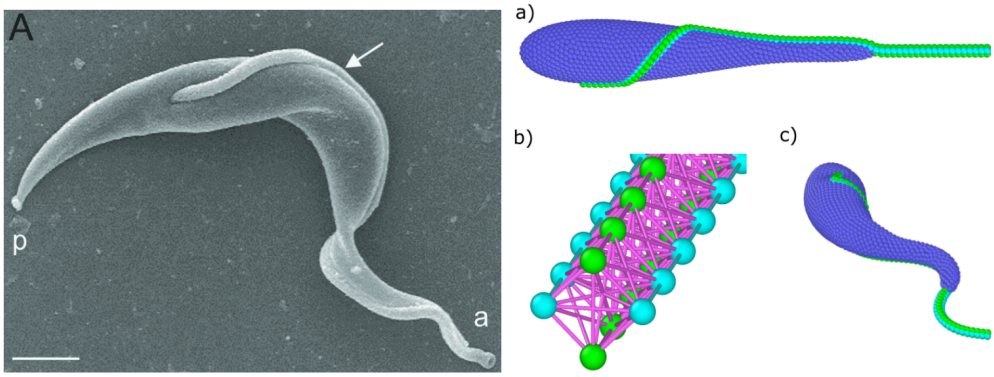
P-081 – Simulating Trypanosome Motility

Florian Overberg

Authors: Dmitry Fedosov, Florian Overberg, Gerhard Gompper

Institute involved in the work: IAS-2

We investigate the motility of the protozoan Trypanosoma brucei (T. brucei) via numerical simula- tions in which a trypanosome model (Fig. 1) is informed by experimental observations [1, 2]. The cell body is represented by a set of vertices distributed homogeneously on a pre-defined elongated surface, forming a triangulated elastic network of springs. This network model incorporates bending rigidity, area conservation, and volume conservation constraints. For the generation of propulsion, a flagellum is attached to the cell body. The flagellum consists of four parallel filaments, two of which are embedded in the body and used for generating a propagating bending wave. We examine the parasite behavior for various conditions, including different flagellum and body stiff- nesses, beating frequencies, actuation wavelengths, and amplitudes. Our simulations yield swimming velocities and rotation frequencies around the swimming axis that are in a good agreement with experi- mental measurements. Additionally, we investigate the importance of various actuation characteristics, such as orientation of the beating plane and the stress-free conformation of the flagellum. We have also started to study parasite motility in a stationary blood suspension, which serves as a first step to understand trypanosome behavior in one of its natural environments such as blood vasculature



References

[1] J. L. Bargul et al., PLoS pathogens, 12, e1005448, 2016 [2] N.Hedergott et al., PLoS pathogens, 8, e1003023, (2012) [3] K. L. Hill, Eukaryotic Cell, 2, p.200-208, (2003)

P-082 – The new version of the Terrestrial Systems Modeling Platform (TSMP2) based on ICON, eCLM, and ParFlow

Stefan Poll, Research Centre Jülich, Germany

Authors: Stefan Poll, Daniel Caviedes Voullieme, Klaus Goergen, Paul Rigor, Stefan Kollet

Institute involved in the work: JSC

Keywords: Simulation

The Terrestrial Systems Modeling Platform (TSMP, github.com/HPSCTerrSys/TSMP2) as regional Earth system model allows to simulate and analyze the complex interactions within terrestrial ecosystems from groundwater to atmosphere. The new version of TSMP, known as TSMP2, is based on a combination of three state-of-the-art models: the next-generation atmospheric model ICON (icon-model.org), a fork of the Community Land Model v5.0 (CLM) with a simplified infrastructure that allows for a more straightforward stand-alone use and model coupling eCLM (github.com/HPSCTerrSys/eCLM), and the integrated hydrology model ParFlow (parflow.org) coupled using OASIS3-MCT (gitlab.com/cerfacs/oasis3-mct).

We present the impact of land-atmosphere coupling approaches on model states, and outline our development strategy along with technical and performance aspects arising from the coupling process. In addition, the performance of this integrated modeling platform is demonstrated through case studies.

P-083 – Advancing Spirit Towards an Atomistic Spin-Lattice Dynamics Framework

Thorben Pürling, Forschungszentrum Jülich

Authors: Thorben Pürling, Stefan Bluegel

Institute involved in the work: PGI-1

Keywords: magnetism, phonons, atomistic spin dynamics, atomistic spin-lattice dynamics

Spirit is an established tool for atomistic spin dynamics (ASD) research and supports a range of important methods that are relevant for calculating properties of magnetic materials. As a set of standard features, Spirit offers implementations of the analytic expressions for energy, generalized force and Hessian to perform dynamical and Monte Carlo simulations as well as stability analysis through transition state theory for magnetic textures [1-2]. Recent interest in coupled spin-lattice dynamics within the magnetism community [3-10] – driven especially by the coupling between magnetic moments and phonon angular momentum – revealed a need to add lattice degrees of freedom to Spirit. With this contribution I showcase the challenges faced and solutions discovered while moving towards extending a feature rich atomistic spin-dynamics code into the domain of conjoint atomistic spin-lattice dynamics while retaining its identity as an ASD research tool.

References

[1] G. P. Müller et al., Spirit: Multifunctional framework for atomistic spin simulations, Phys. Rev. B 99, 224414 (2019). [2] G. P. Müller et al., spirit-code/spirit: New Desktop GUI, update to C++14, [10.5281/ZENODO.7746552] (2023) [3] J. Tranchida et al., Massively parallel symplectic algorithm for coupled magnetic spin dynamics and molecular dynamics, J. of Comp. Phys. 372, 406 (2018). [4] Xufei Wu et al., Magnon and phonon dispersion, lifetime, and thermal conductivity of iron from spin-lattice dynamics simulations, J. Appl. Phys. 123, 085109 (2018) [5] Johan Hellsvik et al., General method for atomistic spin-lattice dynamics with first- principles accuracy, Phys. Rev. B 99, 104302 (2019). [6]Yifeng Wu et al., Atomistic simulations of spin-lattice coupling effects on magnetomechanics in skyrmion materials, Phys. Rev. B 100, 144310 (2019). [7] Pui-Wai Ma and S. L. Dudarev, Atomistic Spin-Lattice Dynamics in Handbook of Materials Modeling, eds. Wanda Andreoni and Sidney Yip, (Springer, 2020). [8] M. Strungaru et al., Spin-lattice dynamics model with angular momentum transfer for canonical and microcanonical ensembles, Phys. Rev. B 103, 024429 (2021). [9] M. Weißenhofer et al., Rotationally invariant formulation of spin-lattice coupling in multiscale modeling, Phys. Rev. B 108, L060404 (2023). [10] Pui-Wai Ma et al., SPILADY: A parallel CPU and GPU code for spin–lattice magnetic molecular dynamics simulations, J. of Comp. Phys. 207, 350 (2016).

P-084 – Summation Compression for Very Low-Rank Adaptation

Alessio Quercia

Authors: Alessio Quercia, Zhuo Cao, Arya Bangun, Richard Paul, Abigail Morrison, Ira Assent, Hanno Scharr

Institute involved in the work: IAS-8

Keywords: Transfer Learning, Parameter Efficient Fine-Tuning

Parameter-Efficient Fine-Tuning (PEFT) methods have transformed the approach of fine-tuning large models for downstream tasks by enabling the adjustment of significantly fewer parameters than in the original model. In this work, we study the “very low rank regime”, where we fine-tune the lowest amount of parameters per linear layer for each considered PEFT method.

By doing so, we reduce the memory consumption and allow for better scaling to big models. Concretely, we propose to compress the input features using their sum: $\sum_{i=1}^{k} x_i$. Our approach can be viewed as rank-1 LoRA update with fixed compression.

Differently from state-of-the-art PEFT methods like LoRA, VeRA, and the recent MoRA, our method uses fewer parameters per layer, reducing the memory footprint and the computational cost. We extensively evaluate our method against state-of-the-art PEFT methods on multiple fine-tuning tasks, and show that our method not only outperforms them, but is also more parameter, memory and computationally efficient. On the Monocular Depth Estimation task using the DepthAnything model pre- trained on the KITTI dataset and fine-tuned on the NYU dataset we show that our method fine-tunes the smallest amount of parameters (comparably to BitFit), while outperforming most PEFT methods in terms of time (except for BitFit), GPU memory consumption (on par with BitFit and MoRA), and Root Mean Square Error (RMSE), being the closest to full fine-tuning.

P-085 – Accelerating bio-plausible spiking simulations on distributed memory

Catherine Schofmann

Authors: Catherine Schofmann, Jan Finkbeiner, Susanne Kunkel

Institute involved in the work: PGI-15

Keywords: spiking networks, simulation, NEST, distributed memory

Introduction The study of long term dynamics in biologically plausible spiking networks depends on systems capable of running large models significantly faster than biological real time. Since CPUs remain the primary target for established simulators, a natural bottleneck at scale caused by the von Neumann design is frequent memory access with minimal compute. Distributed memory architectures, popularized by the need for massively parallel and scalable processing for AI workloads, offer an alternative.

Methods We present an extensible simulator for spiking networks on distributed memory using Graphcore's IPUs. We further implement a custom semi- directed communication algorithm especially suited for distributed and constrained memory environments, which allows a controlled trade-off between performance and memory usage. Spike dynamics are statistically verified by comparison with the same simulations run on a CPU with NEST.

Results Our simulator achieves an acceleration factor competitive with the state of the art at 15x compared to real time for the full-scale cortical microcircuit model on the smallest device configuration capable of fitting the model in memory. The microcircuit model represents experimental connectivity data for 1 mm^2 of cortical tissue, spanning around 300 million synapses, and is considered a building block of brain function. We can achieve further speedup at the cost of lower precision weights.

Discussion With negligible compilation times, the simulator can be be extended seamlessly to arbitrary synapse and neuron models, as well as structural plasticity, unlocking a new class of models for computational neuroscience to simulate efficiently.

P-086 – Transient recurrent dynamics shape representations in mice

Lars Schutzeichel, Juelich Research Centre, Institute for Biological Information Processing (IBI-3)

Authors: Lars Schutzeichel, Jan Bauer, Peter Bouss, Simon Musall, David Dahmen, Moritz Helias

Institute involved in the work: IAS-6 , IBI-3

Keywords: recurrent neural networks; population coding; mean-field methods; information theory; Spin Glass diagrammatics

POF Topic: P2T3: Neuromorphic Computing and Network Dynamics

Different stimuli evoke transient neural responses, but how is stimulus information represented and reshaped by local recurrent circuits? We address this question using Neuropixels recordings from awake mice and recurrent network models, inferring stimulus classes (e.g., visual or tactile) from activity. A two-replica mean-field theory reduces complex network dynamics to three key quantities: the mean population activity (R) and overlaps ($Q^{=}$, $Q^{\neq}$), reflecting response variability within and across stimulus classes. The theory predicts the time evolution of R, $Q^{=}$, and $Q^{\neq}$. Validated in experiments, it reveals how inhibitory balancing governs the dynamics of R, while chaotic dynamics shape overlaps, providing insights into the mechanisms underlying transient stimulus separation. The analysis of mutual information of an optimally trained population activity readout reveals that sparse coding (small R) allows the optimal information representation of multiple stimuli.

Acknowledgements

This work has been supported by DFG project 533396241/SPP2205.

P-087 – Codesign efforts on Modular Supercomputing Architectures in the DEEP-SEA project

Ujjwal Sinha, Jülich Supercomputing Center, Forschungszentrum Jülich

Authors: Ujjwal Sinha, DEEP-SEA WP1 Team

Institute involved in the work: JSC , KU Leuven, KTH, FhG, ECMWF, BSC, CEA

Keywords: Modular Supercomputing Architecture, Optimisation, Energy efficiency, memory management

The Codesign work in the DEEP-SEA project focused on optimising performance, energy efficiency, and memory management across various scientific applications. Benchmarking efforts established automated pipelines and synthetic benchmarks, ensuring system reliability and continuous monitoring. Several applications, including xPic, IFS, FRTM, BSIT, GROMACS, Neko, PATMOS, and TSMP, implemented targeted optimisation strategies to enhance computational efficiency. These efforts included GPU acceleration, hybrid parallelization, dynamic scheduling, algorithmic enhancements, and deep learning integration. Key achievements include improved energy efficiency in molecular dynamics simulations, optimized resource utilization in CFD applications, and advanced performance monitoring techniques. The applications explored methods to efficiently use the Modular Supercomputing Architecture (MSA), paving the way for future advancements in high-performance computing.

P-088 – Search for Stable States in Two-Body Excitations of the Hubbard Model on the Honeycomb Lattice

Petar Sinilkov, IAS-4, Forschungszentrum Jülich

Authors: Petar Sinilkov, Evan Berkowitz, Marcel Rodekamp, Tom Luu

Institute involved in the work: IAS-4

Keywords: Excitons, Hubbard Model, Honeycomb Lattice, Quantum Monte Carlo Simulations, Strongly Correlated Systems, Particle-Hole Excitations

We present one- and two-body measurements for the Hubbard model on the honeycomb (graphene) lattice from ab-initio quantum monte carlo simulations. Of particular interest is excitons, which are particle/hole excitations in low-dimensional systems. They are analogous to the pion in QCD, but without confinement, the question of whether they are bound and stable is of great interest in the condensed matter arena. By measuring one- and two-body correlators across various spin and isospin channels we can compute two-body energies relative to their thresholds, ultimately allowing us to check for stable states.

P-089 – Enhancing Metadata Handling in Research Software

Mustafa Soylu, Forschungszentrum Jülich

Authors: Mustafa Soylu, Stefan Sandfeld, Volker Hofmann

Institute involved in the work: IAS-9

Keywords: fair, metadata, software

Effective management of software metadata is important to ensure their discoverability, reproducibility, and overall quality. This poster introduces two tools designed to simplify and enhance research software development (RSD) metadata management: fair-python-cookiecutter and somesy.

FAIR-python-cookiecutter is a git repository template that provides a structured starting point for Python projects, enabling researchers and developers to integrate metadata effortlessly. It promotes best practices in software development while aligning with key standards such as the DLR Software Engineering Guidelines, OpenSSF Best Practices, REUSE, CITATION.cff, and CodeMeta. The template also incorporates somesy to strengthen the FAIR principles (Findability, Accessibility, Interoperability, and Reusability) of software metadata. In response to user feedback, recent updates have introduced Poetry v2 support, dependency upgrades, and pre-commit tool enhancements, ensuring the template remains a relevant and reliable resource.

Somesy (Software Metadata Synchronization) is a command-line tool that automates metadata consistency across different project files. By supporting formats like CITATION.cff and CodeMeta, it ensures that critical details such as project names, versions, authors, and licenses remain synchronized. This eliminates the need for manual updates, allowing developers to focus on core development tasks. Designed for cross-platform compatibility, somesy works seamlessly on Linux, Windows, and macOS. The latest updates to Somesy introduce, amongst other features, Poetry v2 integration, enhanced validation options, support for ORCID IDs as plain strings, entity (organization) support. We further streamlined metadata handling by Somesy to facilitate post-hoc integration into existing projects.

P-090 – The Joint Lab HiRSE

Robert Speck

Authors: Robert Speck

Institute involved in the work: JSC

Keywords: Research Software, Research Software Engineering

Research software is becoming increasingly important for the success of research and to generate new knowledge, in particular in the fields relevant for the IAS. However, the importance of codes for science has not yet been sufficiently recognized at the national level. Also, the evaluation measures for research are not set in a way that would support sustainable work on research software. Therefore, Research Software Engineering (RSE) is forming as a new subject of investigation, in Europe, Germany and the Helmholtz Association.

Within Helmholtz Information, the underlying HiRSE concept aims at the establishment of central activities in RSE and the targeted sustainable funding of strategically important codes by so-called Community Software Infrastructure (CSI) groups as mutually supportive aspects of a single entity.

In a first “preparatory study”, the innovation pool project HiRSE_PS evaluated the core elements of the HiRSE concept and their interactions in practice over the course of three years. As of October 2024, HiRSE is now the (flexible) Joint Lab “Helmholtz Information - Research Software Engineering”.

For students, researchers and everyone interested in RSE, HiRSE offers many different activities focusing on modern software engineering methods in science, e.g. the HiRSE Seminar Series, Hackathons, an RSE Summer School, and the central website with further resources. In this poster we will present the structure and the achievements of HiRSE, but also the different opportunities for students and researchers working with research software.

P-091 – The Jülich MeteoCloud – A Collaborative Tool

Olaf Stein

Authors: Olaf Stein, Lars Hoffmann, Gebhard Günther, Enxhi Kreshpa, Sabine Griessbach

Institute involved in the work: JSC , ICE-4

Keywords: Data Repository, Community Data

The Jülich MeteoCloud is a collaborative effort of Jülich atmospheric science institutes and JSC to establish a curated science data archive directly connected to and accessible from the Jülich supercomputers. The MeteoCloud is a fundamental basis for simulations and collaborative data analyses in Earth System Sciences. The data is curated by SimLab Climate and ICE-4. It currently serves 200 users from the ESM community with a storage capacity of 4 PByte on the $DATA partition. The data residing on the MeteoCloud is considered as community data which is useful for several compute time projects and for sharing to other collaborators. It consist of three major fractions: 1) meteorological data, which is mostly gridded data from global and regional atmospheric reanalyses, 2) satellite data and other observational data sets, 3) Reanalysis and forecast data from the Copernicus Atmospheric Monitoring Service, 4) Input data for the widely used Climate and Weather Forecast as well as Chemistry Climate models like ICON and MESSy. Moreover, the large data sets are extensively used for training and evaluation with ML methods by the ESDE goup at JSC, e.g, in their projects AtmoRep and HClimRep. Most of the data is of geospatial nature and are stored is stored in space-saving formats that are well recognized in the community like netCDF or grib. It is important to us that the data is enriched with metadata that complies with recognized international standards (like CF conventions).

P-092 – A Multi-Physics Model With Dislocation Induced Nucleation At Grain Boundaries

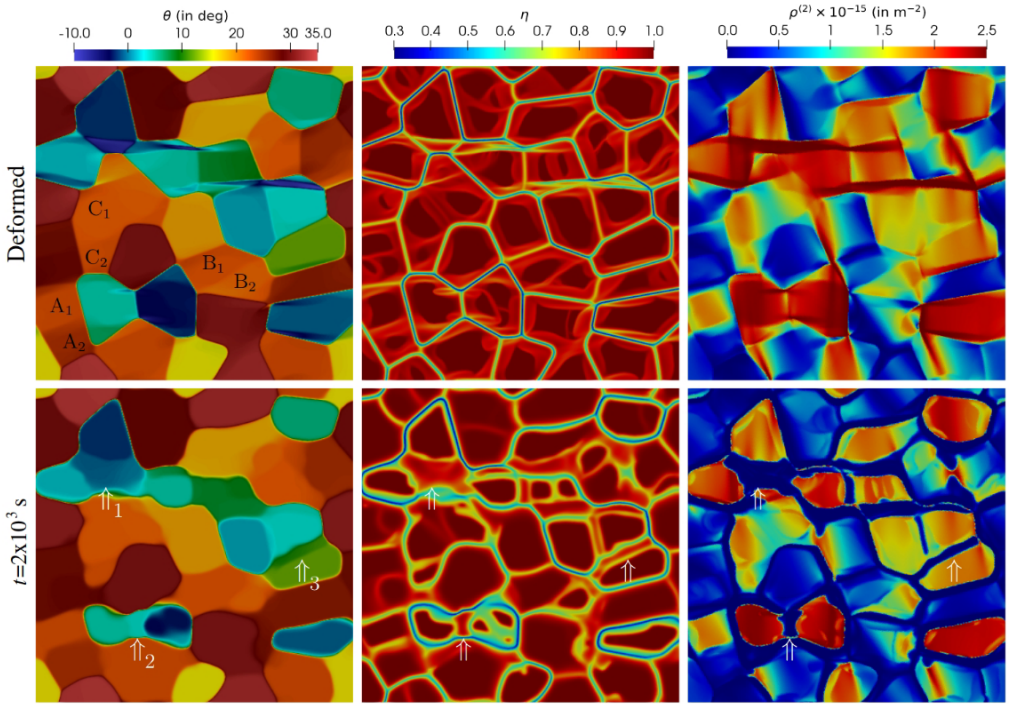
Izzet Tarik Tandogan, Institute for Advanced Simulations – Materials Data Science and Informatics (IAS-9)
Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Authors: Izzet Tarik Tandogan, Michael Budnitzki, Stefan Sandfeld

Institute involved in the work: IAS-9

Keywords: Nucleation, Crystal plasticity, Recrystallization, Phase field, Cosserat

The granular microstructure of metals evolves extensively during thermomechanical treatment by viscoplastic deformation and recrystallization. The grain boundaries can migrate due to increased mobility; severe plastic deformation can result in the formation of subgrains and localized deformation bands. During the heat treatment subsequent to plastic deformation, new dislocation-free grains nucleate, which then grow into the neighboring grains reducing the total energy. Defects such as grain boundaries and second-phase particles are prime nucleation sites due to the strong lattice orientation gradients and the concentration of dislocations at these locations. The numerical modeling of the coupled evolution problem is usually handled with separate specialized frameworks for mechanical deformation and grain boundary migration in a staggered scheme. The nucleation is incorporated as an intermediate step, where nuclei are planted in an ad-hoc manner at possible sites based on trigger criteria such as critical dislocation density, stress, or strain. In this work, we present a unified and thermodynamically consistent field theory, where grains can nucleate spontaneously at pre-existing grain boundaries as a result of plastic deformation. The model couples Cosserat crystal plasticity with a Henry-Mellenthin-Plapp type orientation phase field, which captures curvature and dislocation- driven grain boundary migration. The model's abilities are evaluated based on numerical examples using periodic bicrystals and polycrystals, where strain-induced boundary migration, sub-grain growth, and coalescence mechanisms are observed.



References

[1] Tandogan, I. T., Budnitzki, M., & Sandfeld, S. (2025). A multi-physics model for the evolution of grain microstructure. International Journal of Plasticity, 185, 104201.

[2] Henry, H., Mellenthin, J., & Plapp, M. (2012). Orientation-field model for polycrystalline solidification with a singular coupling between order and orientation. Physical Review B, 86(5), 054117.

P-093 – Overcoming Ergodicity Problems of the Hybrid Monte Carlo Method using Radial Updates

Finn Temmen, IAS-4

Authors: Finn Temmen, Anthony Kennedy, Evan Berkowitz, Johann Ostmeyer, Tom Luu, Xinhao Yu

Institute involved in the work: IAS-4

Keywords: Quantum Monte Carlo Simulations, Hybrid Monte Carlo, Stochastic Simulations, Strongly Correlated Systems,Theoretical Physics, Condensed Matter, Hubbard model

Despite its many advantages, the sensible application of the Hybrid Monte Carlo (HMC) method is often hindered by the presence of large - or even infinite - potential barriers. These potential barriers partition the configuration space into distinct sectors, which leads to ergodicity violations and biased measurements of observables. In this work, we address this problem by augmenting the HMC method with a multiplicative Metropolis-Hastings update in a so-called "radial direction" of the fields, which enables jumps over the aforementioned potential barriers at comparably low computational cost. The effectiveness of this approach is demonstrated for the Hubbard model, formulated in a non-compact space by means of a continuous Hubbard-Stratonovich transformation. Our numerical results show that the radial updates successfully resolve the ergodicity violation, while simultaneously reducing autocorrelations.

P-094 – EBRAINS Infrastructure empowering your ideas

Dennis Terhorst, Forschungszentrum Jülich GmbH

Authors: Dennis Terhorst, Sonja Gruen

Institute involved in the work: IAS-6 , JSC, INM-1

Keywords: interoperability, infrastructure, tools, resources, neuroscience, workflows

POF Topic: P2T3: Neuromorphic Computing and Network Dynamics

The EBRAINS 2.0 Project and the EBRAINS digtal research infrastructure create connections and collaboration on many levels. This poster acts as a starting point for discussions on scientific workflows, available technologies and interoperability between tools, groups, scientific aspects and resources.

References

https://ebrains.eu

Acknowledgements

This project has received funding from the European Union's Horizon 2020 Framework Programme for Research and Innovation under Specific Grant Agreement No. 945539 (Human Brain Project SGA3) and from the European Union's Horizon Europe Programme under the Specific Grant Agreement No. 101147319 (EBRAINS 2.0 Project).

P-095 – Processing very long sequences in biological neuronal networks

Tom Tetzlaff

Authors: Tom Tetzlaff, Markus Diesmann

Institute involved in the work: IAS-6

Keywords: sequences; dendritic action potentials; biological neuronal networks; capacity; spike-train statistics; connectivity

POF Topic: P2T3: Neuromorphic Computing and Network Dynamics

Sensory perception, motor activity generation, language comprehension and production, planning, or solving mathematical equations are sequential processes. Learning, predicting, and recalling sequential data, as well as detecting anomalies in such data streams, are hence fundamental computations performed by the brain. A main challenge in processing such data is context dependency: the correct prediction or recall of an upcoming element in a sequence does not only depend on the previous element, but on the entire history. In [1], we devised an algorithm capable of performing these computations based on a recurrent network of spiking neurons with biophysically interpretable variables and parameters (“spiking Temporal Memory” [sTM]). The sTM algorithm learns complex sequences in a continual, unsupervised manner by means of local synaptic plasticity mechanism known from biology. Prediction and recall of sequence elements are represented by dendritic action potentials. The processing of sequential data in sTM networks is based on ultra-sparse spiking activity, and hence highly energy efficient. So far, the sequence processing capabilities of the sTM algorithm have been demonstrated only for small sequence sets containing few tens of elements. Here, we show that even small sTM networks representing local cortical microcircuits at the sub- millimeter scale can successfully process large sequence sets containing thousands of sequence elements. Mathematical and numerical analysis reveals that the network capacity is primarily limited by the network dynamics in response to unpredicted, ambiguous stimuli. Close to the capacity limit, sTM networks exhibit synapse densities and spiking activity characteristics reminiscent of the neocortex of awake, behaving mammals.

References

[1] Bouhadjar, Y., Wouters, D. J., Diesmann, M., & Tetzlaff, T. (2022). Sequence learning, prediction, and replay in networks of spiking neurons. PLOS Computational Biology, 18(6), e1010233. doi:10.1371/journal.pcbi.1010233

P-096 – Consolidation of top-down modulations balances stability and plasticity

Viet Anh Khoa Tran, PGI-15

Authors: Viet Anh Khoa Tran, Emre Neftci, Willem Wybo

Institute involved in the work: PGI-15

Keywords: dendrites,continual learning,neural plasticity,task modulations

POF Topic: P2T3: Neuromorphic Computing and Network Dynamics

The brain excels at continual learning without catastrophic forgetting - dynamically switching between tasks depending on the current context. On the other hand, conventional machine learning models struggle as weight updates for the current task interfere with previously acquired knowledge. We propose that two biological principles offer a solution to this dilemma: First, neural plasticity primarily occurs without supervision, meanwhile supervised learning in machine learning induces ‘neural collapse’, collapsing same-class inputs to the same network representation, destroying features that might be relevant to other tasks. We instead advocate for self-supervised losses approximating ‘view- invariance’, i.e. learning object-identity from smooth movements. Second, dendritic top-down modulations contextually shape the behavior of feedforward neurons, enabling linearly separability via ‘neural collapse’ for the current task or context. While these paradigms effectively address continual learning for separated tasks (task-incremental), they are not sufficient to explain ‘transfer learning’ between past, present and future tasks. We introduce an algorithm that further optimizes for ‘task-invariance’, implicitly consolidating one-vs-rest modulations into an all-vs-all class-separable representation space. We show that this consolidation algorithm outperforms standard baselines in a class-incremental setup. Furthermore, by adjusting the importance of our consolidation term, we can balance between plasticity and stability depending on e.g. the relevance of the current task. This approach offers a solution to the stability-plasticity dilemma in continual machine learning, while providing a potential explanation on the interaction of feedforward and dendritic top-down modulations for neural plasticity.

P-097 – Combining socio-psychological pedestrian dynamics with AI and simulation tools

Ezel UEsten, Forschungszentrum Jülich

Authors: Ezel UEsten, Anna Sieben, Dilge Dakman, Krisztina Konya

Institute involved in the work: IAS-7

Keywords: Pedestrian dynamics, AI detection, social psychology,

In the *Pedestrian Dynamics – Social Psychology* division at the *IAS-7* we investigate socio-psychological processes that influence pedestrian dynamics, with a focus on how crowds and pedestrian infrastructures are perceived and experienced. To illustrate our interdisciplinary focus at the IAS retreat in May, we chose one of our studies that combines psychological and computational approaches to pushing behavior in crowds. We investigated the conditions under which individuals in a crowd begin to intentionally push on two different levels. On a social level, the question arises as to whether such behaviour spreads through social influence. On an individual level, the role of motivation is to be studied. To address these questions, we developed a manual rating system to code the intensity of forward motion on a 4-point ordinal scale. Using this method on lab datasets, we examined how spatio- temporal factors (e.g., goal proximity) relate to pushing intensity and its local spread. Building on these findings, we explored the feasibility of automatically detecting pushing behavior using AI. Several AI systems analyzed rated video data to detect pushing: first in recorded footage with rough location estimates, then in live streams, and finally at the actor level to pinpoint individuals. Ultimately, this collaboration demonstrates a flow from social psychological coding to the development of a practical tool for crowd management. This tool can be used in real-time interventions, allowing managers to respond (e.g., enlarging areas where pushing occurs) to maintain safety and flow.

P-098 – NUCLEICBERT: DECIPHERING THE LANGUAGE OF NUCLEIC ACIDS

Utkarsh Upadhyay, Forschungszentrum Jülich GmbH

Authors: Utkarsh Upadhyay, Alexander Schug

Institute involved in the work: JSC

Keywords: Bio-Physics, Deep Learning, Structural Biology

In computational biology, determining the 3D structure of biomolecules has been a focal point for many decades. Experimental techniques such as NMR and X-ray crystallography for determining tertiary structures of RNA have limitations due to excessive costs and limited resolution. Although recent advancements in cryo-EM technology have made strides, these shortcomings persist. As a result, various computational techniques have been developed for RNA structure prediction. Deep learning methods have significantly improved protein structure prediction in recent years by utilizing approaches such as convolutional neural networks (CNNs), recurrent neural networks (RNNs), and transformers. However, the direct application of these methods to RNA structure prediction faces challenges due to the limited availability of RNA structure data. While advancements in sequencing technologies have provided an abundance of RNA primary sequence data, the lack of annotated 3D structure data makes it difficult to fully leverage these sequences. To address this challenge, we propose the use of machine learning techniques that can operate with limited training data. Here we introduce NucleicBERT, a language model based on the BERT architecture, specifically designed to predict critical RNA structural features such as contact maps, distance maps, secondary structures, and three-dimensional spatial arrangements. NucleicBERT focuses on the complex relationship between RNA sequence and structure. NucleicBERT's key innovation lies in its precision-focused methodology, which eliminates the need for extensive feature engineering and does not rely on evolutionary information. This model represents a paradigm shift, providing an accurate and versatile tool for analyzing diverse RNA sequences and enhancing computational biology methodologies.

P-099 – Complexity and Criticality in Neuro-Inspired Reservoirs

Michiel van der Vlag

Authors: Michiel van der Vlag, Alper Yegenoglu, Cristian Jimenez-Romero, Abigail Morrison, Sandra Diaz

Institute involved in the work: JSC , INM-6, Universite Paris-Saclay

Keywords: Reservoir computing, The Virtual Brain, Information based metrics

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

Understanding information propagation and computational capabilities in large-scale brain models is crucial for advancing both neuroscience and neuro-inspired computing. By integrating reservoir computing, a recurrent neural network architecture, with The Virtual Brain, a whole-brain simulation platform, a more neurophysiologically-plausible machine learning framework is created. High-performance computing enables a thorough exploration of the vast parameter space, utilizing a diverse evaluation framework that assesses simulations through metrics such as the largest Lyapunov exponent, Detrended Fluctuation Analysis, and the Perturbational Complexity Index, implemented on Graphics Processing Units. This allows for the identification of optimal parameter regimes, a comprehensive characterization of the complex dynamics exhibited by the system, and a deeper understanding of the underlying mechanisms governing the TVB-based reservoir's computational capabilities. Ridge regression, accelerated also by Graphics Processing Units, is used to extract the predictive capacity from the reservoir states. The results suggest that edge-of-chaos dynamics correspond to enhanced memory and prediction accuracy, supporting the potential of TVB-based reservoirs for brain-inspired machine learning.

P-100 – JUPITER - Modular Exascale Supercomputer in Jülich for Europe

Benedikt von St. Vieth

Authors: Benedikt von St. Vieth

Institute involved in the work: JSC

Keywords: JUPITER, Exascale, HPC, AI

POF Topic: P1T2: Supercomputing & Big Data Infrastructures

The poster shows the main building blocks of JUPITER as well as the involved collaboration partners.

P-101 – JUPITER - A Deep Dive into the Core Modules

Benedikt von St. Vieth

Authors: Benedikt von St. Vieth, Andreas Herten, Mathis Bode, Wolfgang Frings

Institute involved in the work: JSC

Keywords: JUPITER, Exascale, AI, HPC, MSA

POF Topic: P1T2: Supercomputing & Big Data Infrastructures

A poster showing technical details about the main JUPITER modules

P-102 – Towards all-electron treatment in electronic structure machine learning

Johannes Wasmer, Forschungszentrum Jülich GmbH

Authors: Johannes Wasmer, Ira Assent, Philipp Ruessmann, Stefan Bluegel

Institute involved in the work: PGI-1 , IAS-8

Keywords: electronic structure, quantum materials, DFT, machine learning, AI

POF Topic: P2T1: Quantum Materials

Electronic structure calculations with density functional theory (DFT) are today the most widely used technique for computational materials design. As materials design enters the artificial intelligence (AI) age, large databases of these calculations, such as the Materials Project, form the basis for creating foundation models. This can be seen in leaderboards such as Matbench Discovery [1]. These AI foundation models mark a paradigm shift in computational materials design since they accelerate the time to solution by orders of magnitude. However, the current DFT databases and AI surrogate models are not accurate enough to design quantum materials. This problem can be solved by employing all-electron, full-potential, fully relativistic DFT, that can reach the required calculation precision. The JuDFT.de codes are among the few established implementations of such methods [2]. They are the only all-electron DFT codes supporting high-throughput data generation that implement the FAIR data guidelines via their plugin integration with the AiiDA.net workflow engine.

We present our progress on the open problem of surrogate AI models for all-electron DFT data for the JuDFT codes. We focus on the JuKKR code, and materials systems with defects, such as magnetically doped topological insulators [3]. We predict the converged electron potential for accelerated DFT, and first-principles exchange interactions for accelerated spin dynamics.

References

[1] Riebesell, J. et al. Matbench Discovery – A framework to evaluate machine learning crystal stability predictions. Preprint at https://doi.org/10.48550/arXiv.2308.14920 (2024). [2] Bosoni, E. et al. How to verify the precision of density-functional-theory implementations via reproducible and universal workflows. Nat Rev Phys 6, 45–58 (2024). [3] Mozumder, R., Wasmer, J., Antognini Silva, D., Blügel, S. & Rüßmann, P. High-throughput magnetic co-doping and design of exchange interactions in topological insulators. Phys. Rev. Mater. 8, 104201 (2024).

Acknowledgements

This work was performed as part of the Helmholtz School for Data Science in Life, Earth and Energy (HDS-LEE) and received funding from the Helmholtz Association of German Research Centres, and from the European Joint Virtual Lab on Artificial Intelligence, Data Analytics and Scalable Simulation (AIDAS). The authors are grateful for the computing time granted through VSR Computing Time Projects on the supercomputer JURECA at Forschungszentrum Jülich (project ID “SuperInt”) as well as computing time granted by the JARA Vergabegremium and provided on the JARA Partition part of the supercomputer CLAIX at RWTH Aachen University (project ID “jara0191”).

P-103 – Research software engineering for the FLEUR code

Daniel Wortmann

Authors: Daniel Wortmann, Gregor Michalicek

Institute involved in the work: PGI-1

Keywords: RSE, FLEUR

At PGI-1, we utilize and further develop the FLEUR software infrastructure to simulate materials properties. Our poster highlights the modern software development techniques we apply to ensure the sustainability and accessibility of our code for both internal and external users. This encompasses development methodologies such as CI/CD, as well as our documentation and user support initiatives.

P-104 – RSE Community? What do I care..

Claire Wyatt, JSC/FZJ

Authors: Claire Wyatt

Institute involved in the work: JSC

Keywords: Research Software, Research Software Engineering

We all just want to get on with our scientific advancements, writing paper, getting grants, you name it. However, for many of us, research software is a key component of our work and writing good code requires quite some effort. A vibrant community can help to reduce this effort, prevent you from re-inventing the wheel, learning from others, and also help you to make all this effort visible.

JuRSE is a FZJ-wide initiative working to raise awareness and increase visibility for scientists who code and looks to improve good practice of research software engineering. We aim to promote the impact on research, highlighting the increasingly critical and valuable role research software and coding serves here. We believe that creating a community will lead to more recognition and professionalisation at the same time as helping those scientists who code to be part of a professional community of practice.

The practice of coding in research is known as ‘Research Software Engineering’ so our community name is Jülich Research Software Engineering = JuRSE.

The poster will show the initiatives and tools that JuRSE has created to engage with the scientists who code at FZJ and (together with HiRSE) within Helmholtz and beyond. It will show how we’re encouraging good practice and researchers to adopt the FZJ software guidelines for research software engineering.

P-105 – Enhancing Monocular Depth Estimation with Multi-Source Auxiliary Tasks

Erenus Yildiz, FZJ/IAS-8

Authors: Alessio Quercia, Abigail Morrison, Erenus Yildiz, Hanno Scharr, Ira Assent, Kai Krajsek, Zhuo Cao

Institute involved in the work: IAS-8 , IAS-6, JSC

Keywords: depth estimation, foundation models, transformers, auxiliary tasks, monocular

Monocular depth estimation (MDE) is a challenging task in computer vision, often hindered by the cost and scarcity of high-quality labeled datasets. We tackle this challenge using auxiliary datasets from related vision tasks for an alternating training scheme with a shared decoder built on top of a pre-trained vision foundation model, while giving a higher weight to MDE. Through extensive experiments we demonstrate the benefits of incorporating various in-domain auxiliary datasets and tasks to improve MDE quality on average by ~11%. Our experimental analysis shows that auxiliary tasks have different impacts, confirming the importance of task selection, highlighting that quality gains are not achieved by merely adding data. Remarkably, our study reveals that using semantic segmentation datasets as Multi- Label Dense Classification (MLDC) often results in additional quality gains. Lastly, our method significantly improves the data efficiency for the considered MDE datasets, enhancing their quality while reducing their size by at least 80%. This paves the way for using auxiliary data from related tasks to improve MDE quality despite limited availability of high-quality labeled data. Code is available at https://jugit.fz-juelich.de/ias-8/mdeaux.

P-106 – Sequence learning under biophysical constraints: a re-evaluation of prominent models

Barna Zajzon

Authors: Barna Zajzon, Younes Bouhadjar, Tom Tetzlaff, Renato Duarte, Abigail Morrison

Institute involved in the work: IAS-6

Keywords: sequence learning; spiking neural networks; biophysical modelling; artificial grammar learning; symbolic representations;

Perceiving causality, anticipating events, choosing actions, and understanding language all depend on processing temporally patterned sequences. Cognitive sciences typically model these processes using symbolic, time-discrete representations. While artificial systems perform well on specific tasks, biologically realistic (spiking) models often focus on isolated features, such as serial order acquisition or temporal rescaling, and rely on architectures tailored to specific functions. This fragmentation makes direct comparison difficult and hinders the identification of shared limitations and possible improvements.

To address this, we introduce a conceptual and computational framework for benchmarking biologically constrained sequence-processing models. Using psycholinguistic paradigms like artificial grammar learning (AGL), we design tasks that assess a broad range of capabilities expected from general sequence processors. The symbolic formulation provides a structured methodology for generating sequences of controlled complexity, enabling systematic and quantitative evaluation across different models. As a proof-of-concept, we apply this framework to compare several prominent models from the past decade.

Testing these models beyond their original scope reveals that while they excel at the tasks they were designed for, they struggle to generalize beyond their intended function. None demonstrated strong performance across multiple features not explicitly included in their initial design. As a result, they fail to provide a sufficiently integrated account of the biophysical mechanisms underlying sequential processing.

Through this meta-analysis, we critically evaluate current models, synthesizing their insights into a set of functional and neurobiological principles. These findings can be corroborated with experimental data and serve as a foundation for guiding future research in sequence processing.

P-107 – All-Atom MCMC Simulation of Protein Folding with ProFASi

Olav Zimmermann, JSC

Authors: Olav Zimmermann, Jan H. Meinke, Sandipan Mohanty

Institute involved in the work: JSC

Keywords: protein folding, peptide aggregation, molecular simulation, Monte Carlo

POF Topic: P1T1: Enabling Computational & Data-Intensive Science and Engineering

We will introduce ProFASi, a versatile open source software for simulation of biomolecular structure formation such as protein folding or peptide aggregation. An all-atom representation of the protein molecules with implicit solvent is used in ProFASi. The software features efficient implementations of several Monte Carlo methods that update the torsional degrees of freedom, as well as global translation and rotation of individual molecules. ProFASi has been used to perform unbiased simulations of protein folding of several small molecules including the designed 92 aa protein Top7 as well as simulation of peptide aggregation up to 512 hexapeptides. Several use cases and options for plugin development are presented.

Presentation of the Institute Divisions

T-01 – Minimal physical modeling of living systems

Thorsten Auth, Forschungszentrum Jülich *and*

Jens Elgeti, Forschungszentrum Jülich

Authors: Thorsten Auth, Jens Elgeti, Dmitry Fedosov, Gerhard Gompper, Marisol Ripoll, Gunter M. Schütz, Gerard A. Vliegenthart

Institute involved in the work: IAS-2

Minimal modeling and high-performance computing can provide important and intuitive insights into the internal processes of living systems. The idea is to use as few ingredients as possible to reproduce the most relevant features of the system under study, and to progressively add details whenever higher complexity is required. We identify the fundamental underlying processes and physical mechanisms of living systems from the cellular scale to tissues and emergent behavior in active matter. Several examples for the research in IAS-2 will be presented, including shapes and fluctuations of active vesicles, microbial motility, blood flow, and cancerous tissue growth. Even though the systems seem to be very different on the first view, the mesoscale simulation techniques are similar, based on particle-based, coarse-grained, and continuum models, and can be combined to study more complex systems. Our results and the obtained knowledge deepen the understanding of generic processes in living matter and allow us to draw connections between different systems.

T-02 – Nuclear Lattice Effective Field Theory in a Nutshell

Fabian Hildenbrand, Forschungszentrum Jülich

Authors: Fabian Hildenbrand

Institute involved in the work: IAS-4

I present Nuclear Lattice Effective Field Theory (NLEFT) as an powerful ab initio approach to calculate the structure of nuclei and nuclear matter. Combining stochastic methods with chiral effective field theory allows the precise calculation over a broad range of the nuclear chart. On top of that the equation of state in neutron stars is accessible. I will present the ongoing research program at IAS-4 as well as future perspectives.

T-03 – Engineering topological phases in quantum nanosystems

Lin Wang, Forschungszentrum Jülich

Authors: Lin Wang

Institute involved in the work: IAS-4

The ability to engineer topologically distinct materials opens the possibility of enabling novel phenomena in low-dimensional nano- systems, as well as manufacturing novel quantum devices. As an introduction to this topic, we show how the symmetries of the one- dimensional Su-Schrieffer-Heeger (SSH) model lead to chiral topological insulators and demonstrate how defects within this system can be used to engineer topological localized states at exactly zero energy. We then extend our example to a more realistic and stable system: the atomically precise one-dimensional graphene nanoribbon. Our findings show how careful inclusion of defects, either point or line, can be advantageous in engineering topological materials. This presents a promising route to engineering topological phases in quantum nanosystems.

T-04 – Introduction to IAS-6

Sonja Gruen, FZJ

Authors: Sonja Gruen, Markus Diesmann

Institute involved in the work: IAS-6

The brain is a highly complex organ and ubiquitous in our daily lives. However, little is understood about it or its functions. Undertaking the study of the organ is a challenging and fascinating endeavour and can spawn new technologies and alternative methods of treatment of diseases. Research at the Institute of Computational and Systems Neuroscience (IAS-6) encompasses theoretical, data-analytic and simulation approaches to develop multi-scales models of the brain. It is our firm belief that progress in understanding a complex system like the brain can only be achieved through this multi-faceted approach. Research at IAS-6 is not an endeavor conducted in single working groups but an interactive effort combining different expertise in one common scientific area - computational neuroscience across the five working groups. Our research follows a scientific loop - data from experimental partners is analyzed and feeds into simulation as well as model development. Theories are formed and lay the foundation for the design of new experiments together with the results from modeling. Also, experimental data from new experiments can be predicted and in a new round, models can be validated against such data once they become available. As all steps involve the handling of big amounts of data, data management and the set-up of analysis workflows is also a focus of the institute. All research performed follows the open science strategy to share research data and software.

T-05 – Physics of AI

Moritz Helias

Authors: Moritz Helias

Institute involved in the work: IAS-6

Methods of artificial intelligence progressively enter all fields of science as well as many areas of everyday life. Yet the principles by which neural networks attain their impressive capabilities of information processing are still to be understood. The reason is that they acquire their function not by design, but by a process of training that adjusts a large number of parameters in response to the presented training data – these parameters undergo a process that is formally equivalent to an interacting many particle system. As a consequence, methods from statistical physics enable us to shed light into the collective phenomena that control learning and inference. We here present recent results based on this physics-inspired approach with regard to expressivity of neuronal networks, their ability to learn features from data, and the prediction of the effect of architectural choices on network performance.

T-06 – Shaping the Future of Crowd Safety: From Flames to Footsteps

Lukas Arnold *and*

Mohcine Chraibi, IAS-7

Authors: Lukas Arnold, Mohcine Chraibi

Institute involved in the work: IAS-7

At our institute, we look at civil safety in many different ways, combining the study of fire, how people behave, and how people walk. Our research aims at how fires start, how smoke spreads, and how it affects visibility, which is iias-7 mportant for getting people out of danger. But safety is not just about physics; it's also about psychology. How do people behave when they can't see well, an alarm sounds, or they are unsure of what is happening? To understand these situations, we combine experiments, data analysis, and modeling at different levels – from fluid dynamics to crowd behavior. We develop open-source tools, design large-scale experiments, and collect real data to improve simulations and inform safety strategies. This talk will explain how our joint research goals will create the next generation of safety systems that can assess, predict and respond to hazards.

T-07 – Retrieval of sun-induced plant fluorescence from hyperspectral imagery

Jim Buffat, Forschungszentrum Jülich

Authors: Jim Buffat

Institute involved in the work: IAS-8

Accurate estimation of solar-induced fluorescence (SIF) from hyperspectral remote-sensing data is crucial for assessing plant photosynthesis. Various techniques have been developed for SIF retrieval, with growing interest in physical approaches due to upcoming satellite missions like ESA's FLEX. Our novel method integrates physical radiative transfer principles and self-supervised neural networks to retrieve SIF in the O2A band. This method shows good agreement with established methods and in-situ measurements. Additionally, it demonstrates local adaptations and first-order diurnal SIF variation.

T-08 – Galaxy Morphology Classification with Counterfactual Explanation

Zhuo Cao, Forschungszentrum Jülich

Authors: Zhuo Cao

Institute involved in the work: IAS-8

Galaxy morphologies play an essential role in the study of the evolution of galaxies. The determination of morphologies is laborious for a large amount of data giving rise to machine learning-based approaches. Unfortunately, most of these approaches offer no insight into how the model works and make the results difficult to understand and explain. We here propose to extend a classical encoder-decoder architecture with invertible flow, allowing us to not only obtain a good predictive performance but also provide additional information about the decision process with counterfactual explanations.

T-09 – Materials Data Science and Informatics

Stefan Sandfeld

Authors: Stefan Sandfeld

Institute involved in the work: IAS-9

In this presentation, an overview of some of the IAS-9 activities will be given. This covers both the machine learning and data science activities as well as the activities concerning research data and knowledge engineering.

T-10 – The Futures of Computing at JSC

Robert Speck

Authors: Robert Speck

Institute involved in the work: JSC

The Jülich Supercomputing Centre (JSC) is at the forefront of Europe's high-performance and quantum computing initiatives, shaping the future of supercomputing and artificial intelligence. In this talk I will highlight the different aspects of JSC's mission, from HPC to quantum computing, from cutting edge simulations to artificial intelligence, from education to research. I will shed light on JSC's integrated support infrastructure with its domain-centric Simulation and Data Labs (SDLs) and cross-sectional Algorithms, Tools and Method Labs (ATMLs), as well as on selected community services.

T-11 – Computational Biomedicine - Developing and using molecular simulation, machine learning, and bioinformatics tools to investigate neurotransmission in the human brain

Giulia Rossetti, INM-9/IAS-5 and JSC

Authors: Giulia Rossetti

Institute involved in the work: INM-9

Uncovering key molecular aspects of chemical neurotransmission, namely how neurons interact with each other, is a required ingredient to understand how the human brain works. It is also fundamental to decipher how drugs act upon the central nervous system, so far, unfortunately, mostly unknown. Biomolecular simulation is an excellent tool to address these issues. Within this context, our Institute (INM-9/IAS-5) develops and applies multi-scale biomolecular simulation methods (from quantum to coarse- grain) to investigate key events at the synapses, from the release of neurotransmitters in the pre-synaptic neuron to their binding to neuroreceptors (such as G-protein coupled receptors) at the post- synaptic cleft. Quantum mechanical processes involved in neurotransmission (such as proton transfer and enzymatic catalysis) are being investigated using our massively parallel Quantum Mechanical/Molecular Mechanical (QM/MM) interface (called MiMiC, https://mimic-project.org). A significant fraction of our work is in collaboration with experimentalists, and it is capitalized to develop neuro-active ligands and neurotracers for neuroimaging of the brain and supported by AI methods, in collaboration with colleagues from Juelich and RWTH-Aachen University and beyond.

T-12 – An IAS perspective on the Peter Grünberg Institut 1 - Quantum Theory of Materials

Gregor Michalicek, FZJ

Authors: Gregor Michalicek

Institute involved in the work: PGI-1

Calculating properties of crystalline solids and surfaces by simulation tools is a crucial ingredient for understanding and guiding related experiments. In this context ab-initio methods like density functional theory or the GW approximation to many-body perturbation theory and related property calculators have become an indispensable approach. Conceptualizing new phenomena or following the scientific quest of the international community, in the Peter Grünberg Institut 1 we develop and employ such tools as part of a simulation infrastructure for the investigation of complex structural, electronic, magnetic and transport quantities of quantum materials - for fundamental research and practical applications, especially in the field of materials for information processing, neuromorphic and quantum computing. Depending on the application use case the program packages can be used either manually or by automatized workflows on computer architectures ranging from desktop workstations up to the GPU-accelerated exascale infrastructure JUPITER, enabling unique research opportunities. By means of high- throughput calculations the tools can also be used to generate large amounts of data for statistical and AI approaches to tackle research questions. In this talk the Peter Grünberg Institut 1 is introduced. The main developments FLEUR, Spex, juKKR, and Spirit are shortly sketched and some lighthouse research results are highlighted.

T-13 – Neuromorphic Principles for Self-Attention

Emre Neftci, Forschungszentrum Jülich

Authors: Emre Neftci

Institute involved in the work: PGI-15

The causal decoder transformer is the workhorse of state-of-the-art large language models and sequence modeling. Its key enabling building block is self-attention, which acts as a history-dependent weighting of sequence elements. Self-attention can take a form strikingly similar to synaptic plasticity, which can be efficiently implemented in neuromorphic hardware. So far, challenges in deep credit assignment have limited the use of synaptic plasticity to relatively shallow networks and simple tasks. By leveraging the equivalence between self-attention and plasticity, we explain how transformer inference is essentially a learning problem that can be addressed with local synaptic plasticity, thereby circumventing the online credit assignment problem. With this understanding, self-attention can be further improved using concepts inspired by computational neuroscience, such as continual learning and metaplasticity. Since causal transformers are notoriously inefficient on conventional hardware, neuromorphic principles for self-attention could hold the key to more efficient inference with transformer-like models.

Presentation on Large Research Projects and Infrastructures

T-14 – JUPITER - Pushing Technical and Scientific Boundaries to the Exascale Level

Benedikt von St. Vieth

Authors: Benedikt von St. Vieth

Institute involved in the work: JSC

With the availability of the “JU Pioneer for Innovative and Transformative Exascale Research” (JUPITER), a unique research infrastructure for the European HPC and AI community is made available. With an tremendous amount of compute and storage capacities and capabilities, the installation of them accompanied at the early stages via the “JUPITER Research and Early Access Program” (JUREAP), a large amount of applications have been used to enable research on the system with day one. This talk will give highlights from the installation of the system, enriched by information and insights from JUREAP, and future plans for the “JUPITER AI Factory” (JAIF).

T-15 – Better Software Better Research

Claire Wyatt, JSC/FZJ

Authors: Claire Wyatt, Robert Speck

Institute involved in the work: JSC

A growing number of people in academia are combining their research expertise with programming and are practising research software engineering on a regular basis in their role. The research software that results from this work is a key component of research and should be considered a research output in its own right. It is also vital that the practice of research software engineering continues to improve to meet centre and Helmholtz quality standards. Over the past two years, two projects have been promoting the importance of research software and the quality standards for research software engineering at FZJ and across Germany. This talk will cover the goals and initiatives of both HiRSE (Joint Lab Helmholtz Information - Research Software Engineering) which functions at the Helmholtz level and our own JuRSE (Jülich Research Software Engineering) Community of Practice at FZJ. These two projects work closely together to encourage good practice, raise awareness of the important role of research software and the visibility of those creating the software.

T-16 – Fostering interdisciplinarity: The Jülich Neuromorphic Computing Alliance

Abigail Morrison, IAS-6 Forschungszentrum Jülich

Authors: Abigail Morrison

The Jülich Neuromorphic Computing Alliance (JUNCA) was established in November 2022 to strengthen the links between researchers in neuroscience, materials science, computer science, electrical engineering, and physics in FZJ through the coordination of collaborative activities and the establishment of efficient communication. In this talk, I will present the history of JUNCA, its achievements in advancing interdisciplinary research into neuromorphic computing at the FZJ, and its future plans.

T-17 – Rhine-Ruhr Center for Scientific Data Literacy - An Introduction and Recent Activities

Katharina Immel, IAS-9 (FZJ)

Authors: Katharina Immel

Institute involved in the work: IAS-9

The scientific landscape is continually shifting towards increasing amounts of data, demanding a greater investment of (time-) resources into the management of these data. As a result, data literacy has become a key element of research for individuals from all domains. Additionally, interdisciplinary, multidisciplinary, and collaborative approaches, as well as identifying synergies between different data- literacy related initiatives are more essential now than ever before. The DKZ.2R focuses on a combined methodological data literacy, combining data science and machine learning skills, high performance computing and research data management competencies. Our main objective is to promote a holistic methodological data literacy, offering support for researchers to break through data related hurdles in order to find cross-domain solutions and synergies. The regional focus of the DKZ.2R allows us to offer in-depth support, making resources more generally available and facilitating connections between researchers and research groups across institutions and domains. Our overall aim is to support data literacy for researchers from all over Germany, while ensuring high quality in all of our offerings. This mixture of in-depth and more general long- and short- term solutions allows us to promote a holistic data literacy while constantly adapting to the challenges of a changing scientific landscape. In this talk we will introduce the services of the DKZ.2R and highlight recent and upcoming events that are relevant to members of the IAS.

T-18 – Helmholtz AI Consulting - supporting AI innovation in Helmholtz

Stefan Kesselheim, FZ Jülich

Machine Learning is gaining pace in many fields in science. In order to support this, Helmholtz has created the platform Helmholtz AI, which - among other things - offers consulting. In “exploration consulting”, the consultant teams interact with scientists throughout the Helmholtz research fields on the conceptual level. We discuss use cases, strategies, models, datasets etc. and provide external input to ongoing or planned AI projects. In “realization consulting” we jointly develop a prototype solution that shows that an approach is viable. The talk introduces the concept with examples. Maybe a starting point for a collaboration?