Fred A. Hamprecht

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I work on principled machine learning for the natural sciences. Trained as a quantum chemist and drawn, by way of spatial statisics, into machine learning, I spent well over a decade building machine learning methods for bioimage analysis that led the international connectomics benchmarks. In 2023 I pivoted my entire laboratory back to quantum chemistry and the centennial problem of orbital-free density functional theory; in 2026 that program was awarded an ERC Advanced Grant. I have enjoyed moving between fields and am happy to see them converge in Scientific AI.

POSITIONS

since 2008	Full Professor (W3), Heidelberg University
2001–2008	Associate Professor (C3) for Multidimensional Image Processing, Heidelberg University, appointed at the age of 26
2001	PostDoc, Seminar for Statistics, ETH Zürich
1998–2001	Dr. sc. nat., Physical Chemistry, ETH Zürich. Advisors: Wilfred van Gunsteren, Walter Thiel
1993–1998	Chemistry at ETH Zürich, EPF Lausanne, Imperial College London and the University of Cambridge

INTERNATIONAL APPOINTMENTS AND VISITS

2025	Sabbatical at Physics Department, University of Edinburgh
2019–2020	Guest Professor for Artificial Intelligence, Uppsala University
2014–2015	Weston Visiting Professor, Weizmann Institute of Science, Rehovot
2012–2017	Visiting Scientist, HHMI Janelia Research Campus
2007–2011	Affiliate Professor of Pathology, Children's Hospital, Harvard Medical School

ACADEMIC SELF-GOVERNANCE AND INSTITUTION BUILDING

since 2024	Member of the AI Board of Heidelberg University
since 2023	Member of the Board of Directors, Interdisciplinary Center for Scientific Computing (IWR)
2020–2023	Vice Dean, Department of Physics and Astronomy
2020–2022	"Pandemic" Dean of Students. I designed and implemented measures that gave students the greatest possible participation through the closures
2008–2020	Initiator and co-founder of the Heidelberg Collaboratory for Image Processing (HCI), an industry-on-campus center. I drove the effort that brought it into being and secured large parts of its funding (around 10M€ total) from the Excellence Initiative and Bayer, Bosch, Sony, Zeiss as well as SMEs. With four chairs and around 100 members it was then Germany's largest academic image processing center, and a pioneering template for public-private partnership
2013–2018	Director of the CellNetworks Math-Clinic Core Facility for bioimage analysis
2007–2010	Head of the Technical Platform, Viroquant Research Centre for Systems Biology of Virus-Cell Interactions

MACHINE LEARNING AT HEIDELBERG

I secured funding for a newly created full ML professorship, established ML as a second pillar alongside modeling, simulation and optimization at my institute, and helped eventually merge these pillars into scientific AI. I founded the mlai.uni-heidelberg.de platform and networking series (2023), created the physics MSc specialization "Computational Physics" (2013) and drove the creation of a new physics MSc core course on "Machine Learning and Physics" (2022).

SERVICE TO THE RESEARCH COMMUNITY

Ongoing	Reviewing proposals for DFG, ERC, and for national research funders of Belgium, the Czech Republic, Denmark, Israel, Luxembourg, Norway and Singapore
2024	Organizer, Dagstuhl seminar on "Low-Dimensional Embeddings of High-Dimensional Data"
2020	Initiated and ran data-against-covid.org, a volunteer data-scientist platform
2015	Area Chair of CVPR, the leading venue in computer vision and, across all fields, among the most cited publication venues in science
2007	Conference Chair, DAGM 2007, Heidelberg. Further workshops at the Weizmann Institute, in Heidelberg and at ECCV
2004–2014	Steering Committee of the German Association for Pattern Recognition (DAGM)

RESEARCH FUNDING

ERC Advanced Grant (2026) for machine learning of orbital-free density functional theory. **DFG:** PI in the Excellence Clusters **STRUCTURES** (since 2018) and member of **CellNetworks**; PI in **SFB 1129** (Integrative Analysis of Pathogen Replication and Spread) and **SFB 1134** (Functional Ensembles); PI in **RTG 1653** (Probabilistic Graphical Models) and **RTG 2581** (Morphodynamics); several individual grants. From 2007 to 2019 a Principal Investigator in the Heidelberg Graduate School of Mathematical and Computational Methods for the Sciences under the Excellence Initiative. Further support, from 2012 to 2018, from HHMI Janelia.

SELECTED RESULTS

- **Quantum Chemistry and scientific AI.** As an MSc student in Cambridge I parametrized the HCTH exchange–correlation functional (*J. Chem. Phys.* 1998), which found wide use. Twenty-five years later, KineticNet (*J. Chem. Phys.* 2023) and its successors took the first serious steps towards a transferable, learned kinetic energy functional; ours is today the most accurate and robust across molecular systems (JACS 2025).
- **Connectomics.** I formalized the reconstruction of neural wiring diagrams from electron microscopy as signed graph partitioning and built solvers — among them the mutex watershed — for it (*Nature Methods* 2017). They held the top of the CREMI and ISBI 2012 leaderboards for the better part of a decade, brought significant HHMI funding to Heidelberg, and set the bar for the later industrial-scale efforts of Google and the US BRAIN Initiative.
- **Essentially no barriers in neural network energy landscapes** (ICML 2018). The textbook picture of isolated local minima is false: sufficiently wide and deep networks have connected minimum manifolds. This helps explain why deep networks can be trained at all, and is influential today well beyond optimization.
- **Steerable CNNs.** I introduced the notion of a steerable neural network layer in my MSc course and set it as a term project; the resulting paper (CVPR 2018) is one of the founding contributions to geometric deep learning in computer vision.
- **What UMAP actually optimizes.** With Sebastian Damrich I showed that the purported loss function of the most widely used non-linear dimension reduction method is not the one it actually optimizes, derived the correct one, and established its close relation to contrastive learning (NeurIPS 2021, ICLR 2022).
- **Optimal lattices for sampling** (*IEEE Trans. Inform. Theory* 2005): the definitive answer to how best to sample a high-dimensional stochastic process on a finite budget.
- **The algebraic path problem for graph metrics** (ICML 2022): a unification and generalization of the important graph distances.
- **ilastik.** Conceived, cross-funded and led by me from 2008 to 2018, before my former student Anna Kreshuk at EMBL took over. It brought interactive machine learning to wet-lab biologists — 60,000 downloads in the past twelve months, some 3,900 citations (ISBI 2011, Nat. Methods 2019), over twenty person-years of development — and set the paradigm that Fiji, CellProfiler and QuPath subsequently adopted. Its usefulness helped create dedicated funding instruments for machine learning in bioimaging at the Chan-Zuckerberg Initiative, de.NBI and Horizon Europe.

RECOGNITION

ELLIS Fellow (since 2020) and Fellow of ELIZA, the DAAD Konrad Zuse School of Excellence in Artificial Intelligence · "40 leading scientists under 40" (*Capital*) · Scholar of the Studienstiftung des deutschen Volkes (1993–1998). My group took first prize at the MICCAI Brain Tumor Segmentation Challenge 2014 and held the top of the CREMI (2016–2025), ISBI 2012 (2016–2019) and SNEMI3D (2016) connectomics leaderboards, with best-paper awards at DAGM 2008 and 2013, MLMI 2012 and GCPR 2018. h-index above 60.

TEACHING, TRAINING AND REACH

- My lecture recordings on machine learning and image analysis have been viewed a cumulative million times.
- Nine former PhD students now hold professorships at Universities and Universities of Applied Sciences including Zürich, Potsdam, Dresden, Odense. One alumna leads a group at EMBL, and many more head groups and departments at Bosch, Siemens, Bayer, Zeiss, Philips and Amazon.
- In 2020 my group carried out the image analysis for the Baden-Württemberg "Kinderstudie", which showed that children were not drivers of the pandemic and underpinned an early reopening of kindergartens and schools.

SCIENTIFIC PATH

My first scientific love was quantum chemistry. I started working in the lab of Walter Thiel during my undergraduate degree in chemistry, and moved to Cambridge for my MSc thesis with Nick Handy. For the PhD, I opted to return to Zürich to work under the joint supervision of Wilfred van Gunsteren and Walter Thiel to study the quantum dynamics of enzymatic proton transfer. The project entailed a high-dimensional nonlinear optimization problem (the reparametrization of MNDO).

Attracted by the immaturity of high-dimensional optimization, I started working on high-dimensional experimental design / Bayesian optimization and the optimal sampling of stochastic processes. This work fell more into the realm of Applied Mathematics, and led to a short PostDoc at the Seminar for Statistics at ETH. Given my expertise in high-dimensional sampling, I was almost immediately appointed to an Associate Professorship in "Multidimensional Image Processing" at Heidelberg University at age 26.

The professorship was endowed by the Robert Bosch company: from 2001 to 2008, I spent much of my scientific quality time consulting for Bosch in machine vision for quality control. It was a thorough schooling in what industry genuinely needs from research, and the experience that later allowed me to conceive and build the Heidelberg Collaboratory for Image Processing (HCI). When the endowment period came to an end, I returned to the unbridled study of fundamental questions.

From 2010 on the lab managed the rare feat of publishing state of the art methods in first-tier machine learning and computer vision conferences, all the while solving fascinating applied problems in bioimage analysis, which were crucial for advances in the neurosciences and developmental biology. From ca. 2018 onwards, computer vision benchmarks started to be dominated by network architectures trained on ever larger data sets which had to be curated manually. Not much enthralled by that perspective, I started looking for more fundamental questions, making contributions to problems such as branched optimal transport or algebraic graph theory.

Most notably, however, I remembered that eminent problem first encountered during my MSc thesis: finding an orbital-free kinetic energy functional of the density. Equipped with all that I had learned about machine learning in the intervening time, I decided to give that old problem a new push. Greatly encouraged by our initial results which outperformed the state of the art on our first attempt, I decided to pivot the entire lab to machine learning for quantum chemistry in the fall of 2023. In hindsight and propitiously, my scientific path has equipped me with some of the requisite very diverse skills, and I am now burning to help achieve a centennial dream: orbital-free DFT.