STRUCTURES | NEWS

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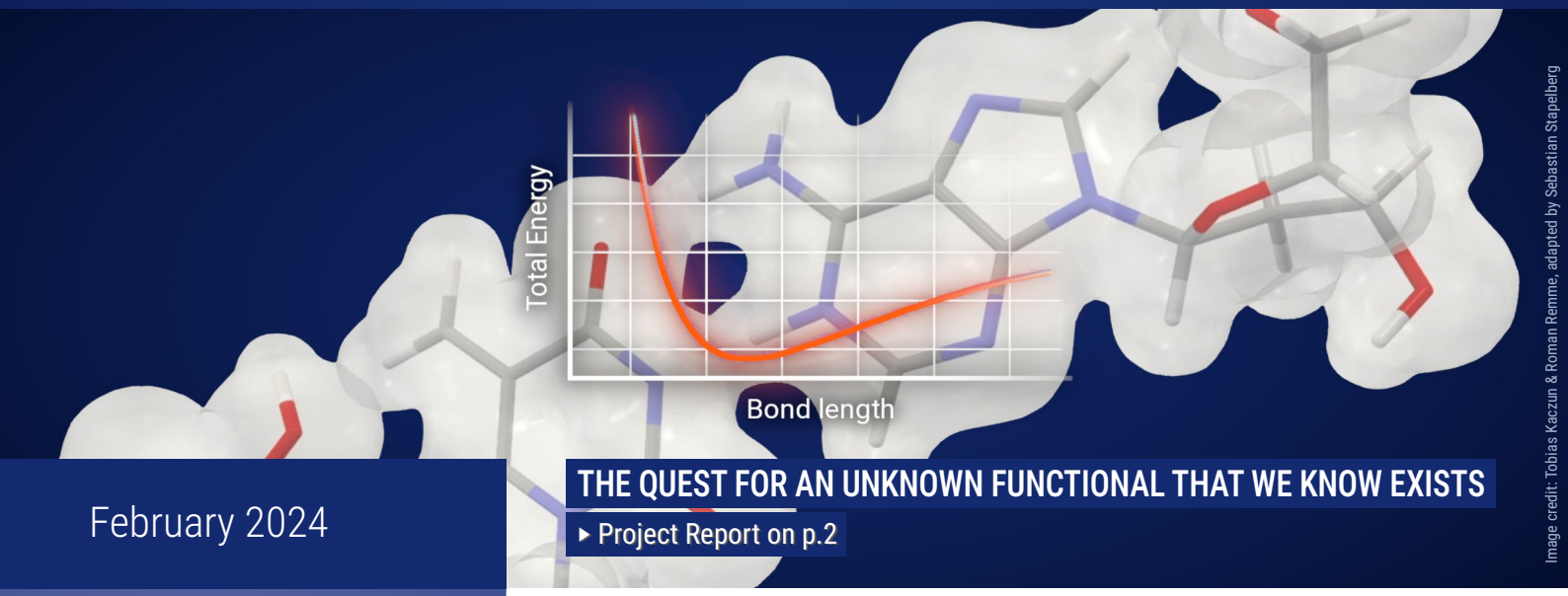

Image credit: Tobias Kaczun & Roman Remme, adapted by Sebastian Stapelberg

THE QUEST FOR AN UNKNOWN FUNCTIONAL THAT WE KNOW EXISTS

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February 2024

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Upcoming

- **Feb 9:** Jour Fixe: Dominika Wylezalek
- **Feb 19:** HI4AI in Medicine
- **Feb 21:** EP Math & Data event: *Tea, Coffee, Cake and TDA: Persistent Homology for high-dimensional data with Sebastian Damrich* (Start: 2pm)
- **Apr 25:** Machine Learning Galore!
- **May 21-24:** Chemical Compound Space Conference (CCSC2024)

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BRIEF NEWS

Probing Universal Dynamics with Topological Data Analysis in a Gluonic Plasma

Quark gluon plasmas (QGP) refer to an exotic state of matter formed under extreme conditions, such as those found in high-energy nuclear collisions at LHC or microseconds after the big bang. In a QGP, quarks and gluons are no longer confined within hadrons but exist freely in a hot medium.

In a novel study, a German-Austrian research team led by STRUCTURES member Jürgen Berges has explored the non-equilibrium time evolution of an initially over-occupied gluonic plasma. The team employed advanced SU(2) lattice gauge theory simulations alongside persistent homology – a sophisticated mathematical method for identifying topological features – to analyze the plasma. Their research uncovered universal patterns, exposing a cascade of energy that repeats itself within the QGP. This phenomenon, known as self-similarity, offers deeper insights into fundamental physics and the early universe.

The application of persistent homology provides a fresh perspective on, and a clearer picture of, the plasma dynamics. Persistent homology extracts topological structures from point clouds of data, features measures of their dominance and can be sensitive to extended structures of varying sizes in the data.

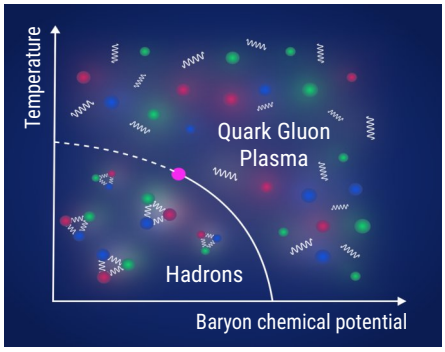


Fig. 1. *Sketch of the QCD phase diagram*

Moreover, non-local excitations, including topological defects such as eddies in a fluid, can be important for a wide range of dynamical phenomena ranging from heavy-ion collisions to ultracold quantum gases. Beyond that, higher-order correlation functions are numerically hard to access but can contain important information in strongly correlated systems. The study opens a new pathway for their characterization including topological and non-local quantifiers.

Original Publication:

Spitz, D., Boguslavski, K., and Berges, J., 2023: *Probing universal dynamics with topological data analysis in a gluonic plasma*, *Physical Review D*, doi:10.1103/PhysRevD.108.056016.

PROJECT REPORT

EP 5.4: The Quest for an Unknown Functional That We Know Exists

Invited Article by F. Hamprecht & A. Dreuw (IWR)

What is the kinetic energy of a given ground state electron density? While we know the question holds a significant answer, irritatingly, we do not know how to find it.

When predicting the properties of a molecule, it is possible to simplify by separating nuclear and electronic degrees of freedom. The latter are the subject of *Electronic Structure Theory*, which invokes quantum mechanics to describe the interacting electrons in terms of their many-body wave function $\psi(x_1, \ldots, x_N)$. For sizeable molecules, this is too expensive and instead *Kohn-Sham density functional theory (DFT)* is evoked. The latter models the same system merely via one-body functions $\phi_1(x_1), \ldots, \phi_N(x_N)$ describing non-interacting electrons moving in an effective potential created by the others. Importantly, these functions lead in principle to the exact electron density ρ_{exact}, however, approximations for the unknown exchange-correlation energy functionals need to be made. Although highly successful in practice, Kohn-Sham DFT remains a sort of band-aid solution. Why?

In the 1960s, Hohenberg and Kohn made a tantalizing discovery: for systems in their electronic ground state, knowledge of the electron density alone suffices to compute the exact electronic ground state energy, and wave functions or "orbitals" are not needed! To find the ground state electron density, one minimizes its overall energy in the potential created by atomic nuclei. The overall energy has, of course, a kinetic contribution stemming from the kinetic energy density functional $E_{kin}=T[\rho_{exact}]$. Vexingly, it has so far been impossible to identify the functional $T[\rho]$ yielding the exact kinetic energy of a given ground state electron density.

Being able to do so is not only of great theoretical interest: it paves the way for variationally optimizing the electronic ground state

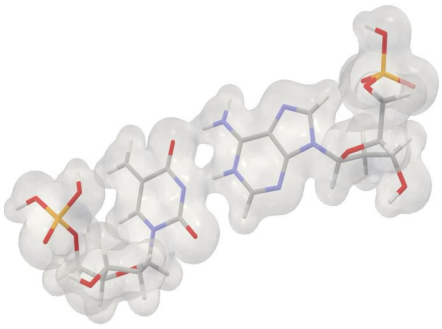


Fig. 1. *Electron density isocontour of a DNA base pair. The sticks serve as a simplified representation of 'bonds.' The truth lies in the electron density.*

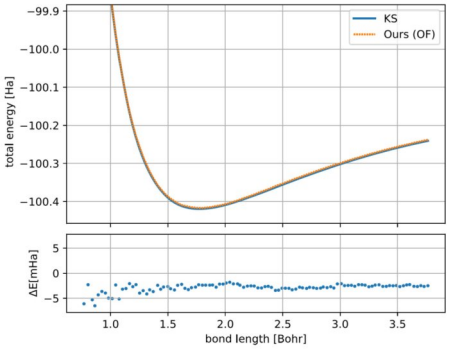


Fig. 2. *A small heureka moment: energy of the H_2 molecule as a function of distance, the first binding curve we reproduced without orbitals.*

density without taking recourse to the much more complicated many-body wave functions. This sixty-year old promise, called *pure* or, more contemporarily, *orbital-free* DFT, promises computing molecular properties with a complexity growing merely linearly with system size.

Our Exploratory Project (EP) has set out to make good on this old promise. We are encouraged by the observation that in important parts of chemical space, interactions exhibit a degree of *locality*: a change in one position will propagate only by a few bond lengths, not across long ranges. Thus we are confident that the kinetic energy functional, whose analytical description has remained elusive, can be learned from a finite training set. The second piece of good news is that we can create arbitrary amounts of ground truth using accurate, albeit more costly, quantum chemical procedures. And finally, machine learning has progressed with great strides. We now possess the necessary algorithmic building blocks and hardware for the task.

The learning machinery has at least two interesting aspects. First, our learning algorithms are guaranteed to respect the symmetry of the problem. A consequence is that old friends from mathematical physics play their role – to guarantee *SE(3) equivariance*, we learn spatial filters whose angular parts are required to be spherical harmonics. *Clebsch-Gordan coefficients* help construct tensor products between such filters and tensorial features. Second, unlike most supervised machine learning, we do not seek to predict the outcome (here: a ground state electron density for a given set of nuclei positions). Instead, we learn to predict the objective, which in turn is minimized to yield a ground state electron density.

In early 2023, three years of stubborn and often challenging work finally paid off: our learned kinetic energy functional was good enough for density optimization in two-electron systems, and gave kinetic energies with the required accuracy in small hydrides. This was a worldwide "first", and we are now working to enable it for larger systems.

Indeed, the EP has taken on a life of its own. Roman Remme, who initially worked alone on what was a high-risk project, now co-advises an enthusiastic group of students. The insights from theoretical chemistry proved pivotal, with Tobias Kaczun making vital contributions nudged by Andreas Dreuw asking the right questions. Fred Hamprecht is so captivated by the project that he is refocusing (and renaming) his lab around this endeavour. Maurits Haverkort and Björn Malte Schäfer are set to join, and we are much looking forward to working with them!

Original Publication:

Remme, R., Kaczun, T., Scheurer, M., et al. 2023: *KineticNet: Deep learning a transferable kinetic energy functional for orbital-free density functional theory. J. Chem. Phys.*, doi: 10.1063/5.0158275.

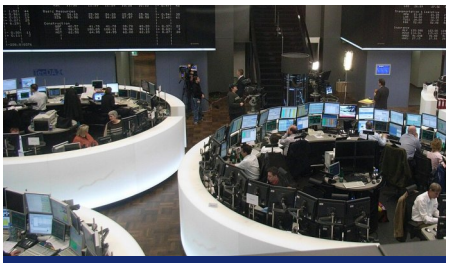
STRUCTURES COLLEGE

STRUCTURES Welcomes its First YAM Fellows

We are delighted to introduce *Richarlotte Razafindravola* and *Olivette Tchouangnou Chuagua* as our inaugural *STRUCTURES-YAM Fellows* under the *Young African Mathematicians (YAM)* Fellowship Programme. During their two-semester research stay, the two students, who joined in October, engage in a rich academic programme including courses, seminars and research projects. Their work is under expert supervision by Felix Joos, Roland Herzog, Hans Knüpfer & Robert Scheichl, ensuring a comprehensive and supportive learning environment. Additionally, YRC students Louise Kluge and Maximilian Siebel provide invaluable mentorship.

YAM is a collaboration between the *African Institute for Mathematical Sciences (AIMS)* centres in *Cameroon, Senegal, Rwanda, Ghana and South Africa*, and notable German excellence clusters *(Hausdorff Center Bonn; Mathematics Münster; MATH+ Berlin; STRUCTURES)*. The fellowship programme aims to empower talented AIMS students by enabling them to undertake research stays in Germany. This unique opportunity allows them to collaborate with international experts, enhancing their skills and expanding their academic and professional networks.

For this newsletter edition, we interviewed Olivette Tchouangnou Chuagua and Richarlotte Razafindravola about their scientific journey, expectations and aspirations.



Source: Wikipedia/DesertEagle

In December, the two YAM fellows took part in a field trip to the German Stock Exchange organized by *Upstream*, the network for women* in STEM at the HGS Math-Comp and IWR.

Interview with Olivette Tchouangnou Chuagua:

Olivette Suzy Tchouangnou Chuagua

What motivated you to apply for the YAM Fellowship?

I am passionate about mathematics, and I applied for the YAM fellowship to be able to learn from leading experts, collaborate with diverse peers, and contribute to advancing mathematics in Africa and beyond. I am impressed by the many opportunities the programme offers, and by its international research environment.

What are your expectations for your research stay in Germany?

My long-term goal is to become a leading mathematician in modelling and numerics, enabling me to contribute to the sustainable development of Cameroon and Africa. During my visit, I plan to establish new collaborations, research projects and to expand my professional network. Moreover, I look forward to immersing myself in German culture and language.

What fascinates you about mathematics?

Mathematics reveals the hidden patterns and structures of the universe. It allows me to explore abstract concepts and apply them to real-world problems. Mathematics also challenges me to think creatively and rigorously and to appreciate the beauty and elegance of mathematical proofs. I enjoy learning new concepts and techniques and discovering connections to other fields.

What advice would you give other students considering similar opportunities?

My advice to other students is *to go for it!* Don't be afraid to challenge yourself and explore new areas of learning. You will gain valuable skills, experiences and connections that will be helpful. It is also a lot of fun and a rewarding experience. So do not hesitate and apply for the opportunity that suits you best!

Interview with Richarlotte Razafindravola:

Richarlotte Valérà Razafindravola

What motivated you to apply for the YAM Fellowship?

First of all, I would like to thank the STRUCTURES Cluster of Excellence of the Universität Heidelberg for giving me this opportunity. I applied for the YAM Fellowship Programme because of my passion for mathematics and the desire to contribute to African mathematical research.

What are your expectations for your research stay in Germany ?

My research stay in Germany is an open door for me to conduct in-depth research and collaborate with experts in the field of Discrete Mathematics. I believe that interacting with experts of Discrete Mathematics will strengthen my knowledge so that I will be ready for a further education position (PhD).

What fascinates you about mathematics?

Mathematics, to me, is the core of all scientific fields. If we are not able to understand it, then it will be hard to understand the rest.

What advice would you give other students considering similar opportunities?

For students eyeing similar opportunities, I advise them to embrace curiosity and approach challenges without fear. Every obstacle is a chance to learn and grow, making the journey as valuable as the destination.

STRUCTURES COLLEGE:

The STRUCTURES-YAM fellowships are hosted within STRUCTURES College, an academic unit dedicated to cross-career & cross-discipline interaction, international exchange, and the unity of research & teaching.

STRUCTURES INTERVIEWS

STRUCTURES Asks: Freya Jensen and Victoria Noel (EP Math & Data)

The EP 1.4. "Math & Data" is one of STRUCTURES' earliest Exploratory Projects. In this interview, the project's managing team, Freya Jensen (IWR) and Victoria Noel (ITP), give an overview of its activities and aims:

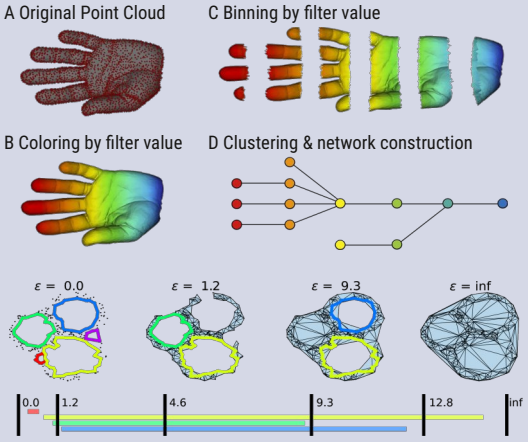
What is topological data analysis and why is it significant?

The goal of *topological data analysis* (TDA) is extracting significant topological features from data, providing insights into the global structure of datasets. Essentially, it serves as a generalization of clustering methods.

One of the most well-known tools from the TDA toolbox is *Persistent Homology* (PH). In addition to finding clusters in datasets, it also allows us to investigate holes and *d*-dimensional voids in the underlying structure of the samples under consideration. Another well-known TDA method is the Mapper algorithm which can be used to visualize the dataset by reducing its dimensionality while most of the topological structure is preserved.

How does TDA connect disciplines?

As the aforementioned techniques can be relatively easily modified to fit different purposes, applications can be found in various fields. The applications of TDA are rather versatile. Method development is one of the cornerstones, where, for instance, pure mathematicians and computer scientists might work together. Such methods can then be used for analyzing data in applied sciences. These include, e.g., astrophysical, physical, biological, medical and material sciences, to name a few. However, TDA has also been applied to network problems of sensor networks and even in social sciences to investigate trends in social networks, including social media. These applied projects also often involve mathematicians as well as researchers from these disciplines, closely collaborating.



◀ *Fig. 1: Illustration of the Mapper Pipeline: A sample is mapped to a lower dimensional space (B), the domain is subdivided into smaller parts (C), connected components of the preimage of one part get the same colour, edges are drawn whenever there is an intersection (D).*

◀ *Fig. 2: Illustration of PH pipeline (dim 1): A filtered simplicial complex is constructed from a point cloud (first line). The barcode represents the "lifetime" of cycles in the complex (second line).*

What is the EP *Math and Data* about?

The EP *"Math and Data"* aims to provide a central point of contact for researchers using topological and geometric methods in data analysis. Over the past four years, different activities were organized by a team of doctoral students to accomplish this.

The EP began with an introductory lecture series in summer 2019, which served as a common ground for future directions and projects. Since the winter term 2019/20, a regular Journal Club has served as a primary meeting point for researchers at Heidelberg University and beyond. Despite the challenges posed by the COVID pandemic, this integral part of the EP has attracted participants from various European universities.

The EP has also hosted workshops annually for an international audience, focusing on the intersection of mathematics and data.

The latest workshop (Sept. 19th–21st, 2023) was dedicated to *"synergies between TDA and life sciences."* Andreas Ott (KIT, Karlsruhe) held the main workshop sessions, offering an introductory course on *algebraic topology and persistent homology*, followed by applications in his coronavirus-related research project. Participants primarily had backgrounds in biology, physics, and mathematics. The workshop adopted a hybrid format with over 100 registered participants. We have also organized two online colloquia within the workshop, successfully inviting renowned researchers in the field: Kathryn Hess (EPFL) and Anthea Monod (Imperial College London).

As for the future, we wish to explore more topological and geometric data analysis techniques, especially the ones used in the machine learning community. Our upcoming events will revolve around this area.

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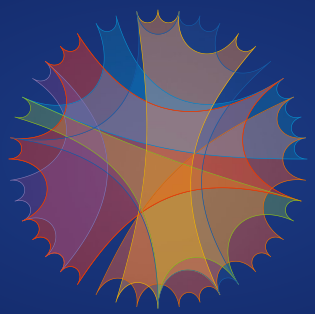

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