# DASHH Matchmaking Workshop 2025 (April 28th, 2025)

**Participants:**
***DASHH Management***: Edgar Weckert (former DASHH IB Chair and Photon Science Director, Kaus Ehret (DASHH coordination), Heike Hufnagel Martinez (DASHH coordination), Christiane Ehrt (DASHH coordination), Sabine Le Borne (DASHH spokesperson), Nina Rohringer (DASHH spokesperson)
***DASHH PIs and Scientists***: Alexander Itin (TUHH), Martin Kliesch (TUHH), Matthias Mnich (TUHH), Maximilian Kiener (TUHH), Pierre-Alexandre Murena (TUHH), Linnea Hesse (UHH), Winnifried Wollner (UHH), Nils Margenberg (HSU), Sadia Bari (DESY), Yannis Schumann (DESY), Christoph Heyl (DESY), Michael Kolbe (HZI)

## Matchmaking Profiles of DASHH PIs/Scientists

Domain Sciences:
https://www.dashh.org/people/matchmaking_profiles/domain_sciences/index_eng.html

Applied Mathematics:
https://www.dashh.org/people/matchmaking_profiles/applied_mathematics/index_eng.html

Computer Science:
https://www.dashh.org/people/matchmaking_profiles/computer_science/index_eng.html

## Domain Sciences

### Nina Rohringer

- X-ray free electron laser sources
- non-linear X-ray matter interaction
- development of novel experimental techniques looking at molecular systems from molecules to solids
- coupled sets of stochastic PDEs, effectively parallelizing, X-ray interaction with particles

### Christoph Heyl

- group leader at DESY
- aspects of ultrafast laser physics and laser technology
- novel photonic methods for ultrafast optics
- one ongoing project with Nihat Ay

- inverse design ⇒ employing approaches of inverse design for developing optical multilayer coatings/structures, using novel inverse design approaches (particularly, ML-inspired inverse design methods)
- photonic partner, multilayer optical design
- acoustic optical principles (acoustic and light waves interaction), looking for potential partners
- typical scenario: certain optic (mirror, optical filter) with certain properties, e.g., glasses with reflective coatings to minimize reflections (demands: broad-band anti-reflective coating that avoids reflection in the visible spectrum)
- find multi-layer stack design and a recipe for this stack with the wished optical properties
- old problem, but classic optimization routines are at their end and finding improvement for targeting this challenge is promising
- intense ultra-sound waves to directly control light (e.g., sound waves in ambient air), simulation efforts to reflect and reshape laser beams, complex shape acoustic waves necessary, what is the necessary reflective index pattern that we have to modulate in that air volume (just starting to enter this topic)
- envisioned methods: very open
- close contact with Sören Laue on the data science side

### Linnea Hesse

- junior professor in the field of biomimetics, UHH
- background: biologist by training, imaging techniques, high-speed video analysis, material property analysis
- questions on how plant functions can help to optimize technical products
- G-fibers function is not well understood, cells can shrink if they take up water / or when they dessicate
- nanocomputer tomography hereon+DESY in combination with digital volume correlation to study cell motion
- missing the step into taking the knowledge of nature into a computer model
- mathematical modeling of plant functions such as motion can help understanding them
- simulation as crucial step for abstracting nature and enabling technical transfer
- state of the art: until now: there are no computational models for G-fibers
- ***presentation link:***

### Michael Kolbe

- CSSB (UHH & HZI)
- structural biologist, bacterial infections, imaging

## Applied Mathematics

### Winnifried Wollner

- professor for Mathematical Optimization

- optimization of systems governed by PDEs
- identification material laws potentially coming from data measurements and the modeling steps in between
- stochastic optimization, particularly coupling of simulation accuracy and requirements for the learning process
- material properties: control of fracture processes, how fracture evolution is governed, also applicable to other material laws
- collaborators: method development collaborating with computer scientists at the University of Hanover
- potential collaboration with HSU
- no focus on specific imaging techniques
- no connections to DESY scientists

### Sabine Le Borne

- professor for numerical mathematics
- mostly linear algebra
- matrices, linear equations, etc.

### Nils Margenberg

- postdoc in the group of Markus Bause
- DASHH alumni
- classical numerical methods combined with neural networks
- optimal control problems quite similar to inverse problems from a computational point of view, our idea: Replace forward model by surrogate model
- results motivates current research: combining numerical methods and hybrid networks eases the computational bottleneck
- collaboration: numerical methods on HPC, devise hybrid classical and neural networks, solve large scale coupled simulations
- (current framework cannot do complex models with coupling)
- ***presentation link:***

## Computer Science

### Maximilian Kiener

- professor for philosophy and ethics (philosopher by training), Head of the Institute for ethics in Technology
- ethics of AI, responsible innovation and sustainability
- explainable AI (e.g., NN)
- data protection, sensitive information
- technical approaches: noise adding
- AI systems working for multiple users (applicability)

- translating ethical principles to be implemented into code (challenge: mathematical principles suited for quantification)
- related to the structure of matter: sustainability, responsible data management, risk management

## Alexander Itin

- worked at Radboud University (Nijmegen, NL), Aalto university (Helsinki), Univ. of Electro-Communications (Tokyo), Hamburg University and TUHH, Space Research Institute (Moscow). https://www.linkedin.com/in/alexander-itin-796117a/
- ML for industry at Bosch Research (Moscow branch, currently being liquidated)
- now temporarily employed at TUHH
- application of classical mechanics and asymptotic methods to various problems
- example: theory for quantum simulators experiments (https://www.fis.uni-hamburg.de/publikationen/detail.html?id=0837b8c8-7c4e-4112-a979-f7a39e2c9641)
- design of photonic crystals and structures (https://papers.ssrn.com/sol3/papers.cfm?abstract_id=4204785).
- numerical methods, ML, finding some analytical design principles
- development of methods for several projects (e.g. https://arxiv.org/abs/2406.08318)
- design of photonic crystals using a geometric approach ⇒ discovery of general principles behind the results of the simulations (https://journals.aps.org/prb/abstract/10.1103/PhysRevB.111.L121404)
- optimal toric packings instead of centroidal Voronoi tessellation (work better)
- not only for photonic crystals, but also for magnetic/plasmonic crystals
- ***presentation link:***

## Yannis Schumann

- working at DESY in IT department
- presenting group on behalf of Philipp Neumann
- high-performance computing and data science at UHH
- one project nearly finished, one project started in particle physics
- development of algorithms or making algorithms more efficient in the context of simulation
- one collaboration with UKE in cancer detection (imaging)
- coupling CFD solver with classical MD simulation
- energy modeling
- offer: knowledge on how to scale algorithms in terms of different types of hardware
- any collaboration topic is interesting

## Martin Kliesch

- quantum computing and related topics
- derive analytical results, analyze algorithms, and provide proofs
- numerical proof of concepts

- also, collaborations with industry and experimentalists
- quantum computing has not been shown to provide better results than classical methods for practically relevant problems yet
- however, large speed-ups for specific problems are expected in the future
- also: quantum-inspired computing:
  1) solve differential equations with Tensor networks
  2) solve QUBO problems (access to Fujitsu's Digital Annealer)

## Pierre-Alexandre Murena

- Junior professor for human-centric ML
- Create AI agents
- Fairness, privacy-preserving aspects
- complementary to Maximilian Kliesch's work but stronger focus on ML
- producing decision-making functions
- humans collected data, this determines the measurements and results
- learning algorithm is curated by humans
- Proper choice of ML is critical and the hyperparameters => super difficult for non-machine learners, but also for machine learners
- used in the real world to solve real-woerld problems
- determine of data selection, choice of ML model is determined by humans
- human user => AI ⇒ model training by AI ⇒ decision-making function as output
- active-learning models ⇒ AI is requesting the human (asked to provide an answer, decision) ⇒ AI is still in control
- idea: AI and human working as a team to solve a problem
- actions: recommendations, actual actions done by AI and human
- AI should take human into account and understand recommendations, decisions, actions
- human trained to design an ML model (e.g., physical situation)
- humans apply modifications, get some quality measures etc.
  => AI suggests modifications
- unlabeled data ⇒ BUT clear opinion on the labels in mind (now what the rules should look like but no time to phrase them) ⇒ interactive clustering loop, AI providing some clustering ⇒ send to human expert to evaluate the clustering ⇒ back to AI, AI will learn and provides a new clustering (learn sth. that humans cannot express)
- Big NN ⇒ understanding the results produced/explanations ⇒ taking the DS of labeled cases and finding rules to describe/explain the outcome
- data completeness-related questions
- translating what people have in mind to mathematical equations
- ***presentation link:***

## Matthias Mnich

- algorithm design and analysis
- complex problems that cannot be solved by formula
- problems: QUBO  problems already mentioned by Kliesch

- complex decision problems
- efficient algorithms ⇒ on large datasets ⇒ understand why algorithms are efficient
- one project with Henry Chapman (crystallography), image data (huge amounts, cannot/need not all be processed, data reduction), actual image has to be constructed from large data, image reconstructions, convex optimization algorithms for image reconstruction