Session of "Fokus Materialchemie" – Thursday, 22.05.2025 13:00 @ Seminarraum BA 05 (TU-Wien, Getreidemarkt 9, BA, OG. 05, BA05G02) join us on ZOOM (ID: 983 0066 2349)



## Heuristically Adaptive Diffusion-Model Evolutionary Strategy

## Benedikt Hartl

benedikt.hartl@tuwien.ac.at

Allen Discovery Center at Tufts University, Institute of Theoretical Physics, TU Wien

Diffusion Models (DMs) represent a significant advancement in generative modeling, employing a dualphase process that first degrades domain-specific information via Gaussian noise and restores it through a trainable model. This framework enables pure noise-to-data generation as well as modular reconstruction of, e.g., images or videos. Concurrently, Evolutionary Algorithms (EAs) employ optimization methods inspired by biological principles to heuristically refine sets of numerical parameters encoding potential solutions to rugged objective functions. Our research reveals a fundamental connection between DMs and EAs through their shared underlying generative mechanisms: both methods generate high-quality samples via structured iterative refinement on random initial distributions. Here, we employ deep learning-based DMs as generative models across diverse evolutionary domains: by iteratively refining DMs with heuristically acquired databases, we can sample potentially better-adapted offspring parameters that are integrated successively into the training of subsequent DM generations. With this, we achieve efficient convergence toward high-fitness parameters while maintaining explorative diversity. DMs also introduce enhanced memory capabilities into EAs, retaining historical information across generations and leveraging subtle data correlations to generate refined samples. In that way, we elevate EAs from procedures with shallow heuristics to sophisticated frameworks with deep memory. Moreover, we deploy classifier-free guidance for conditional sampling at the parameter level to achieve precise control over evolutionary search dynamics to further specific genotypical, phenotypical, or population-wide traits. Our framework thus marks a major heuristic and algorithmic transition, offering increased flexibility, precision, and control in evolutionary optimization processes.