Prof. Dr. P.S. Kousourelakis
Professorship for Data-driven Materials Modeling
TUM School of Engineering and Design

Generative Modeling for Molecules

The development of new drugs relies on the discovery of novel molecules. Conventional methods rely on human expertise and time-consuming experiments to test new molecules. Generative modeling leverages recent advancements in deep learning to tackle the problem of inverse molecular design. Given a set of desirable properties, what set of molecules will satisfy those properties? (*Bilodeau et al. (2022)*)

Project description
This project focuses on the implementation and comparison of different generative modeling strategies. The students will build a small framework of generative models in Python (preferably in JAX) and compare them on standard benchmarks. Students will learn more about numerical simulations, probabilistic programming, and physical systems.

Tasks
The project will include the following tasks:

- Implementation of different generative modeling strategies
- Investigation of performance on popular benchmarks
- Comparison of different methods and strategies
- Literature research

Requirements
- Python programming proficiency (e.g., JAX)
- Interest in machine learning
- Interest in physics simulations

If you are interested in the project or have further questions, please send an email at maximilian.stupp@tum.de.

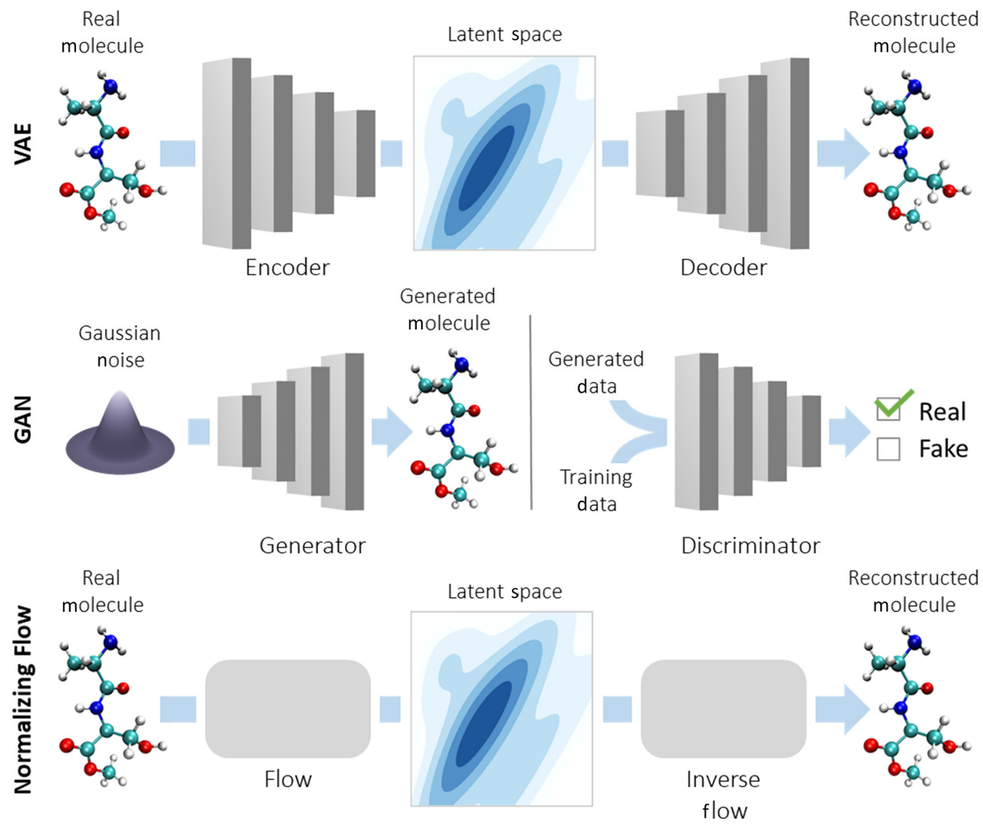

Figure: Comparison of different neural network architectures used in generative modeling. (*Bilodeau et al. (2022)*)