Master's Thesis Project on Inverse Materials Design

Project Description:

We are seeking motivated M.Sc. students to join a cutting-edge research project focused on inverse materials design. This project aims to develop efficient methods for solving the inverse material design problem based on the processing-structure-properties (PSP) linkage (See Fig 1). Considering the

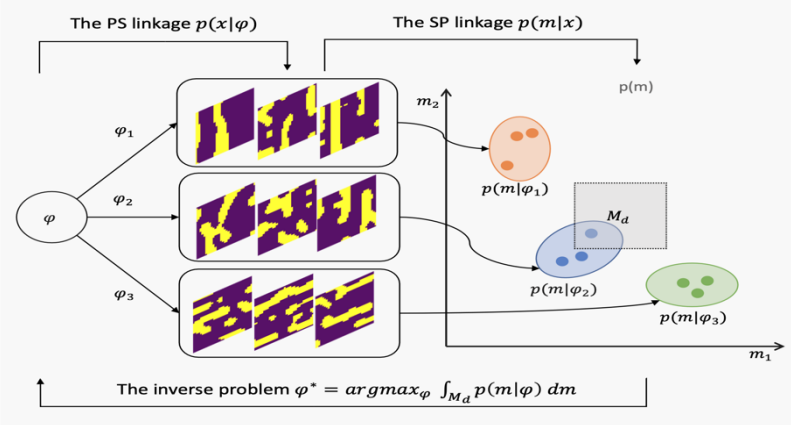

Fig 1: Overview of materials design problem based on inverting the PSP chain: Given a desired property region $\mathbf{M_d}$, the goal is to find optimal process parameters $\boldsymbol{\varphi}$ such that the properties $\mathbf{m}$ of resulting material microstructures $\mathbf{x}$ align as closely as possible with $\mathbf{M_d}$ .The $\boldsymbol{\varphi}$ and $\mathbf{m}$ are connected by the PSP linkage, which comprises two sequential processes: the PS linkage $\mathbf{p(x|\varphi)}$ describing the generation of microstructures $\mathbf{x}$ given process parameters $\boldsymbol{\varphi}$, and the SP linkage $\mathbf{p(m|x)}$ calculating properties $\mathbf{m}$ of microstructures $\mathbf{x}$.

challenging nature of this problem, we will solve this problem in three stages：

S1. **Development of Deep Learning Methods for PDEs**: Utilizing advanced deep learning-based methods such as PINNs and FNOs to efficiently solve the partial differential equations (PDEs) in the structure-properties (SP) linkage.

S2. **Exploration of Continuous Latent Space**: Investigating physically meaningful continuous latent spaces to represent microstructures x , thereby simplifying the high-dimensional discontinuous microstructure space.

S3. **Integration and Inference**: Integrating the solutions from stages 1 and 2 to address the entire PSP linkage and applying Bayesian inference for solving the inverse material design problem.

Skills and Experience Desired:

- Proficiency in numerical methods for PDEs, including finite difference and finite element methods.
- Experience in developing deep learning algorithms, particularly in PyTorch/TensorFlow, or a strong willingness to learn.
- Familiarity with probabilistic statistical methods or a willingness to gain proficiency in this area.

What We Offer:

- Opportunity to work on a challenging and impactful research project with real-world applications.
- Guidance and mentorship from experienced researchers in the field.
- Potential for publication in top-tier academic journals and conferences.
- A stimulating and collaborative research environment.

How to Apply:

Interested candidates can send their CV, a brief statement of research interests and relevant experience (which can be included in the resume or in the email) to **yaohua.zang@tum.de**. Please indicate "Master's Thesis Project Application: Inverse Materials Design" in the subject line.