International Research Training Group IRTG 2657
Computational Mechanics Techniques in High Dimensions

Physics-Based Machine Learning for Inverse Design of Porous Metamaterials

Phu Thien Nguyen, Ludovic Chamoin, Fadi Aldakheel

IRTG 2657 Qualification Year: 01.09.2023 - 31.08.2024
Second Cohort – Doctoral Researcher - Starting Date: 01.09.2024

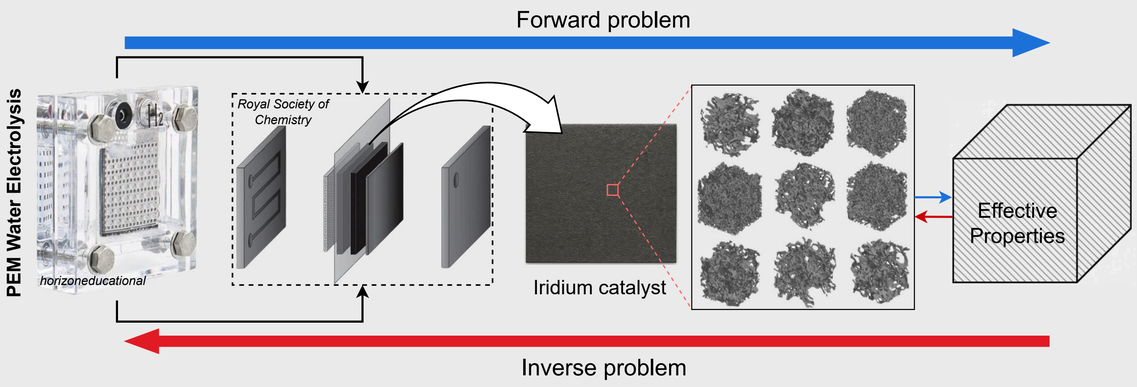
Physics Meets Data-Driven Approaches

For a sustainable economy, mechanical systems must be multi-functional, durable, and consume less energy and material

- Development of novel materials, manufacturing processes, and mechanical systems

Major challenges:

- Multiscale & multiphysics nature of materials, processes, and systems
- Limitations of classical models & numerical methods



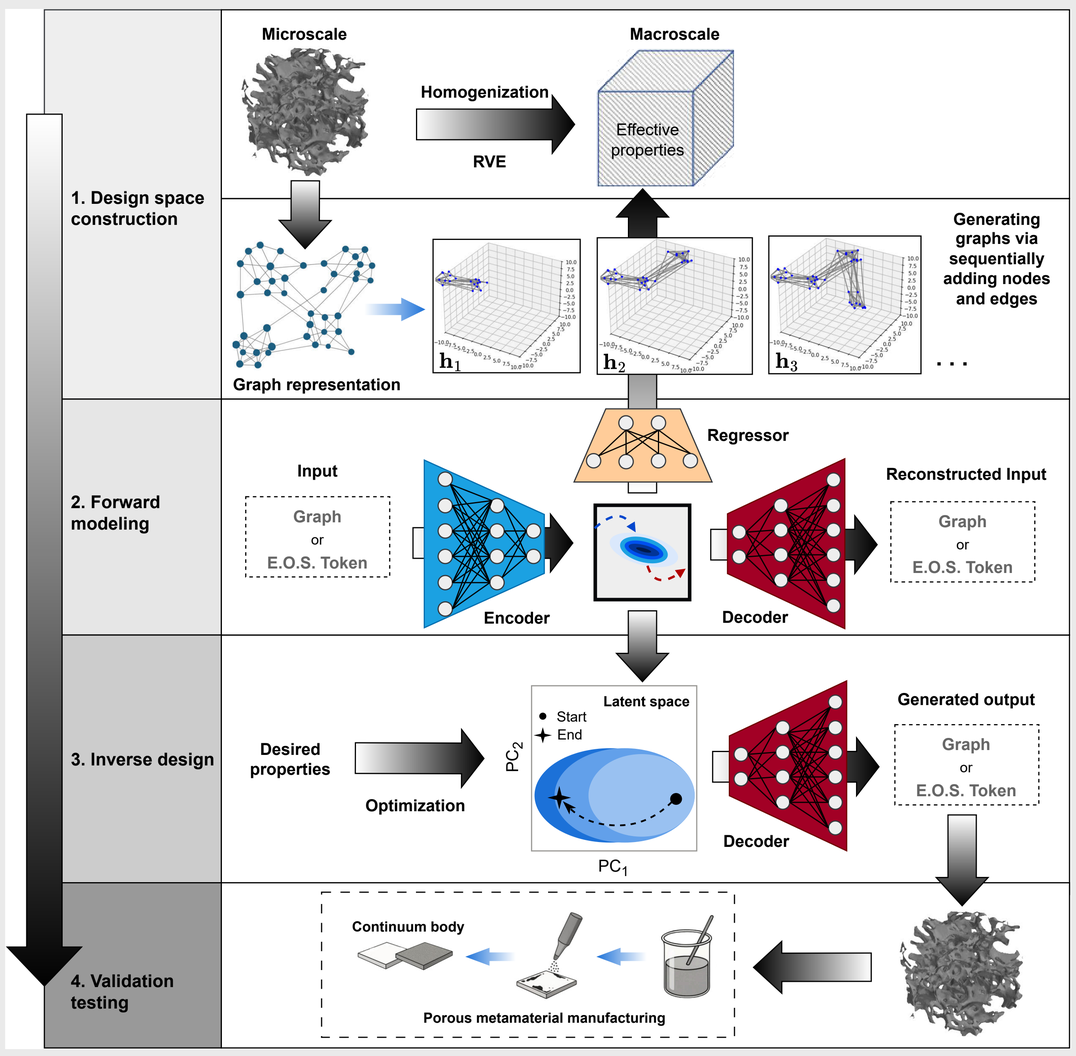
- Forward problem (from micro- to macroscale): **Expensive** high-fidelity computational homogenization
- Inverse problem: **ill-posed** and requires strictly **defined constraints**

Methods

Physics-based ML framework is developed for fast, and cost-effective inverse design of porous metamaterials with tailored properties.

Workflow:

1. **Design space construction**: Microstructures + effective properties
2. **Forward modeling**: Microstructure – property linkages
3. **Inverse design**: Optimization, Classifier-free guidance, ...
4. **Validation**: Fabrication and experimental testing

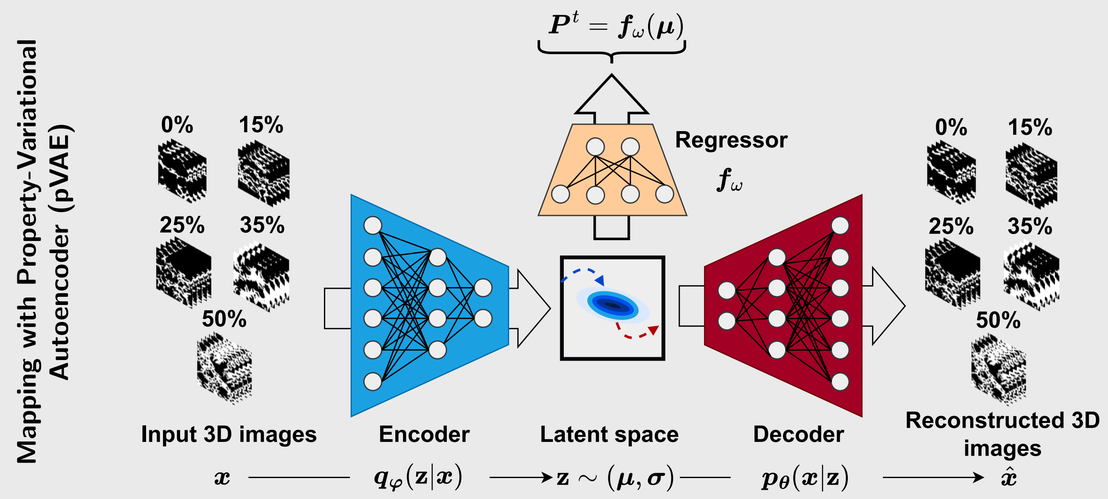


Major goals:

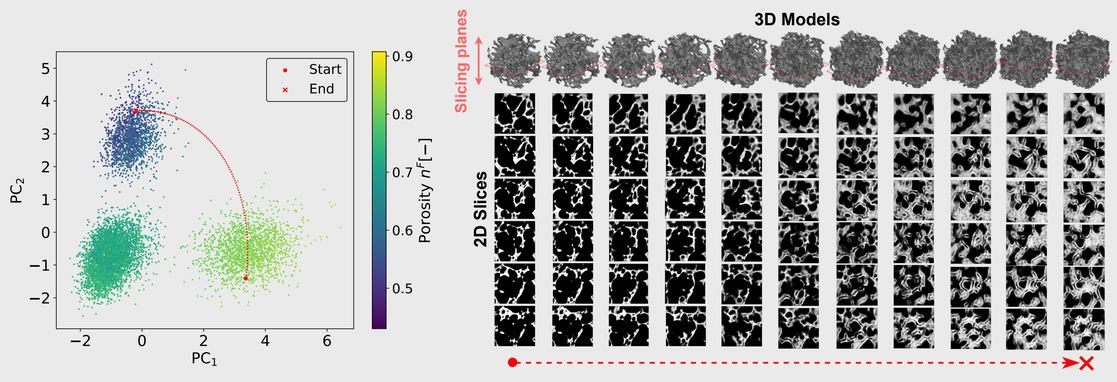
- Design porous metamaterials for multiphysics problems
- Learn underlying probability distribution of microstructures + properties
- Enable variational inference for inverse design

Ongoing Results

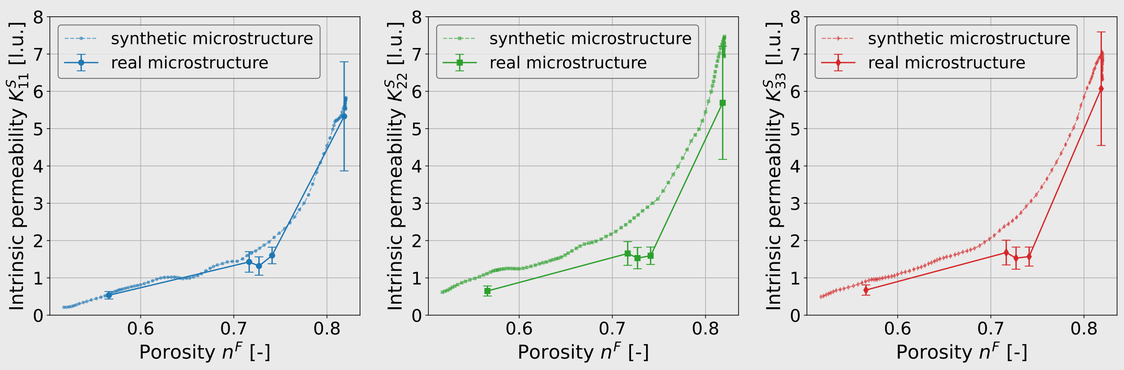
- Testing with CT-scan data from viscoelastic open-cell foam



$$\theta, \varphi, \omega \leftarrow \min_{\theta,\varphi,\omega} \Big[\underbrace{-\mathbb{E}_{q_\varphi(z|x)}\left[\log p_\theta(x|z)\right]}_{\text{reconstruction loss}} + \beta \underbrace{D_{\mathrm{KL}}\left[q_\varphi(z|x) \,\|\, p_\theta(z)\right]}_{\text{Kullback-Leibler (KL) divergence}} + \lambda \underbrace{\left\| P^t - f_\omega(\mu) \right\|^2}_{\text{regressor loss}} \Big]$$



- Accurate microstructure – property mapping yields a smooth, structured latent space, enabling **inter-/extrapolation**



Next Steps

1. **Design space with porous metamaterials for catalyst layer**: Multiphysics → Effective properties + Microstructures
2. **Forward modeling**: Generative model for microstructure – property linkages (Paris-Saclay)
3. **Inverse design**: Multi-objective design (Paris-Saclay)
4. **Validation testing**: From inverse solutions to multiphysics homogenization and experimental fabrication (Paris-Saclay)

Publications

[1] **P.T. Nguyen**, Y. Heider, D. Kochmann, and F. Aldakheel, Deep learning-aided inverse design of porous metamaterials, CMAME, **under review** (2025)
[2] **P.T. Nguyen**, B.-e. Ayouch, Y. Heider, and F. Aldakheel, Impact of Dataset Size and Hyperparameters Tuning in a VAE for Structure-Property Mapping in Porous Metamaterials, PAMM, **under review** (2025)

IRTG Environment and Activities

- ECCOMAS Congress, Lisbon - 2024
- Summer School on Material Design, TU Dresden - 2025 (**scholarship**)
- GACM Colloquium, Braunschweig - 2025
- **Planned stay ENS Paris-Saclay**: September 2026 - March 2027

Université franco-allemande Deutsch-Französische Hochschule
Funded by DFG Deutsche Forschungsgemeinschaft German Research Foundation