3D Multiphase Heterogeneous Microstructure Generation Using Conditional Latent Diffusion Models

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Objective

Develop a fast and flexible framework for generating 3D microstructures with user-defined characteristics, such as volume fractions and tortuosities, to support customizable and efficient material design.

Background

- Microstructures are essential for material performance across ceramics, polymers, and semiconductors.
- Studying structure-property relationships requires a diverse and extensive dataset of microstructures.
- Experimental and statistical methods are expensive, inflexible, and challenging for large-scale generation.

Key Contributions

- Developed a framework for diverse 3D microstructure generation.
- Enabled conditional generation with user-specified volume fractions and tortuosities.
- Integrated manufacturing parameter prediction for generated microstructures.

Methods

Data Preparation

Raw Data:

- Generated 3D simulations of the **Cahn-Hilliard equation** using the Finite Element Method (FEM), varying the concentration field (ϕ) and interaction parameter (χ).
- Over 50 unique combinations of ϕ and χ, resulting in a dataset of 20,000 3D microstructures across 400+ timestamps per combination.

Processed Data: Microstructures are filtered, resized, and thresholded for training.

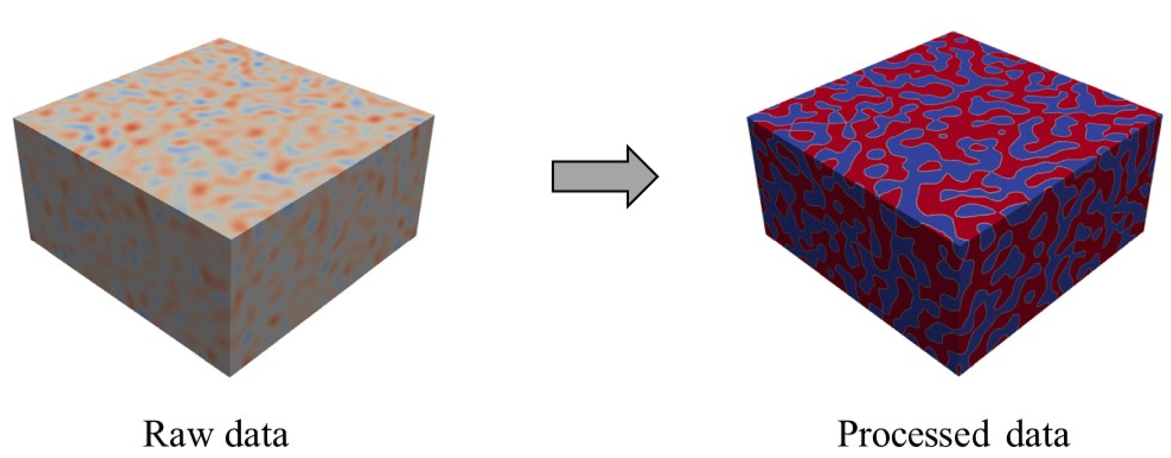

Figure 1. **Data preprocessing:** raw data to processed data

LDM Model Architecture

- **VAE**: Learns optimized latent representations $\mathbf{z}$.
- **Feature Predictor (FP)**: An MLP maps the optimized latent representations $\mathbf{z}$ to ground truth microstructure characteristics.
- **Conditional Latent Diffusion Model**: Generates latent representations of microstructures conditioned on user-defined characteristics.

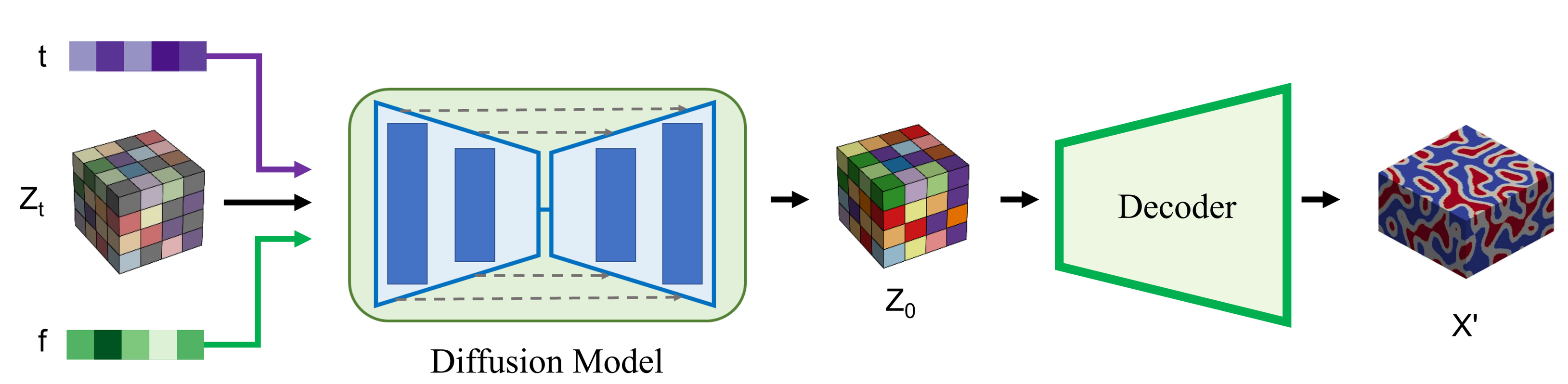

Figure 2. **LDM Inference:** A random Gaussian tensor is denoised using the latent diffusion model (LDM), generating a latent representation $\mathbf{z}$. The pretrained VAE decoder then transforms $\mathbf{z}$ into a microstructure with user-defined characteristics, such as volume fractions and tortuosities.

Results

(a) Predominant phase A - more than 0.5

(b) Predominant phase B - more than 0.5

(c) Predominant phase mixed - more than 0.5

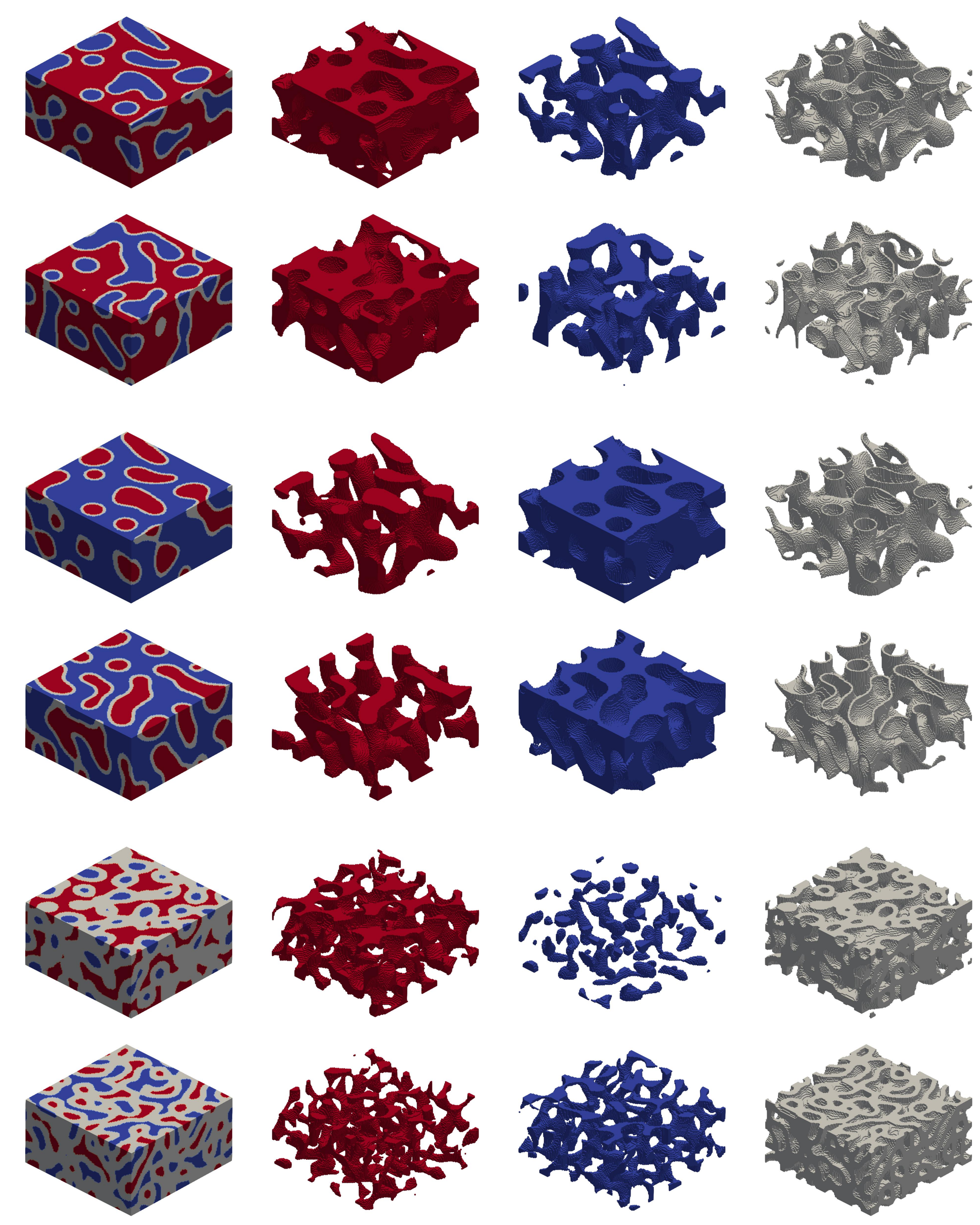

Figure 3. Conditional microstructure generation: Examples of generated 3D microstructures based on user-defined inputs. (a) Predominant phase A (volume fraction > 0.5), (b) Predominant phase B (volume fraction > 0.5), and (c) Mixed phases (balanced volume fractions). For each case, the first column shows the complete microstructure, while the second, third, and fourth columns display thresholded representations of phase A, phase B, and the mixed phase components, respectively.

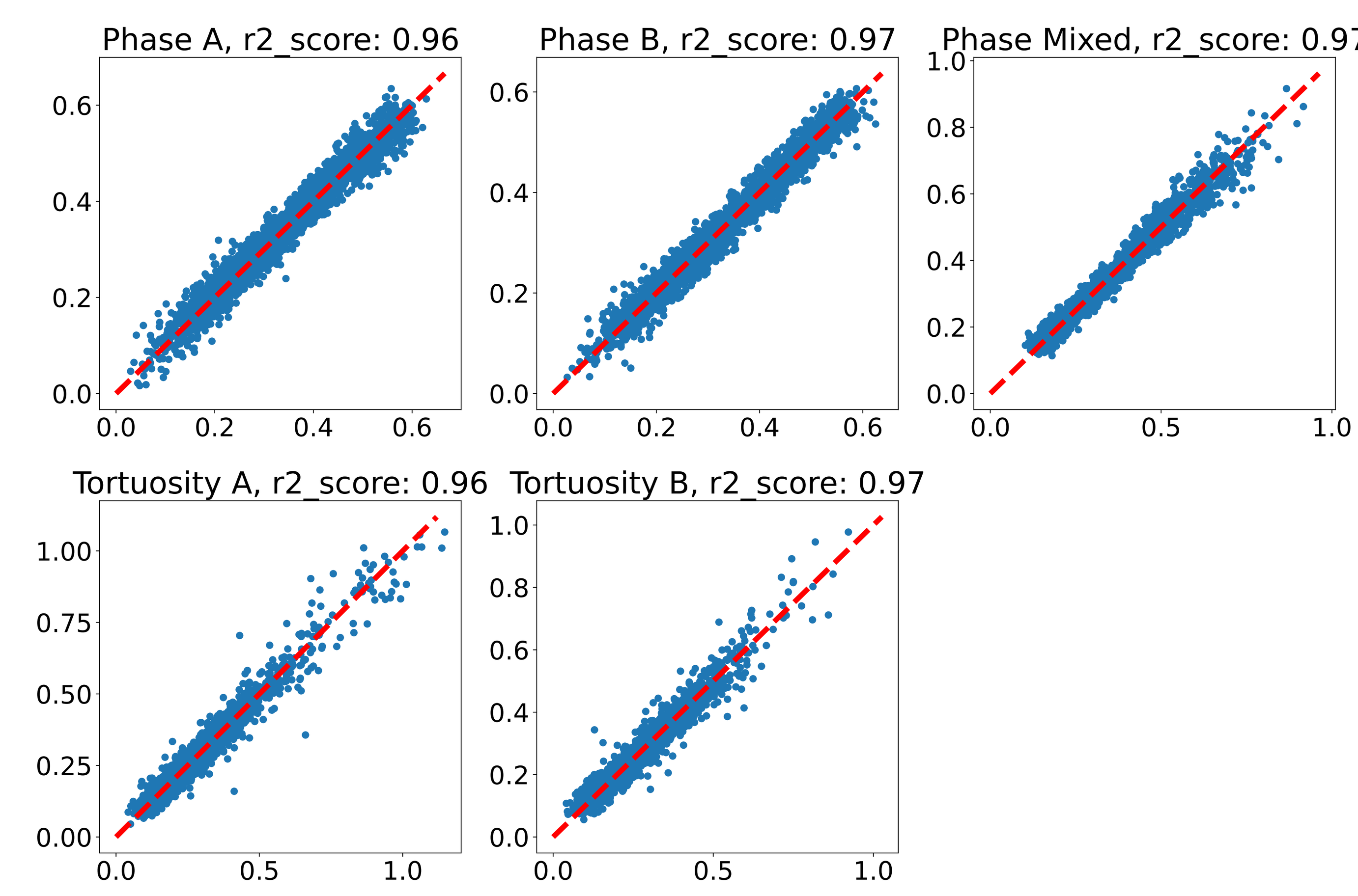

Figure 4. Statistical analysis of conditional microstructure generation: Correlations between all features of interest, user inputs, and the corresponding features measured from generated microstructures.

Conclusions

Key Contributions:

- Presented an **efficient and versatile** Conditional LDM framework for generating customizable 3D microstructures.
- Demonstrated **precise control** over microstructure characteristics, enabling tailored material design.

Future Work:

- Integrate **manufacturing parameter prediction** to bridge design and production.
- Incorporate **experimental data** to enhance realism and applicability.

References

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