Neural Information Processing Systems 2018

PHYSICS-AWARE DEEP GENERATIVE MODELS FOR CREATING SYNTHETIC MICROSTRUCTURES

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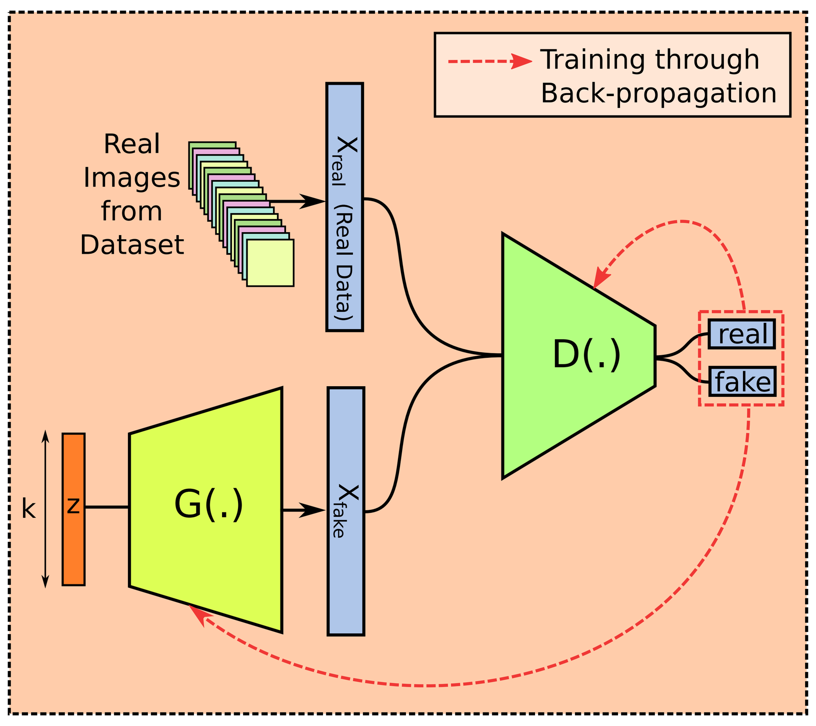
Challenge

- Properties of the material system is intricately connected to the underlying **microstructure**.
- **Microstructure-sensitive design** has been used to tailor a wide variety of properties including strengths, heat and mass diffusivities, lifetime etc. [2,3].
- **Challenge:** How to **synthesize** a **desired** microstructure, given a finite number of microstructure images, and/or some **physical invariances** that the microstructure exhibits?

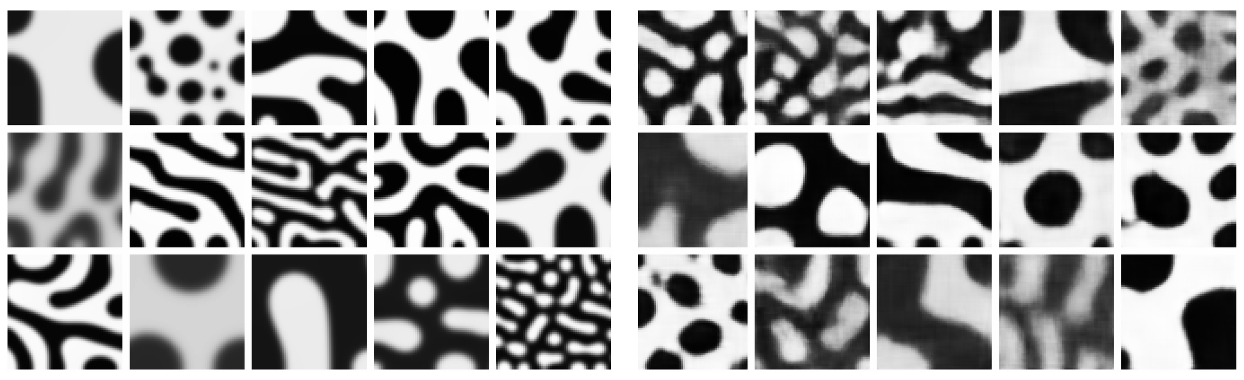
Our Approach

- Our model **explicitly enforces known physical invariances** by replacing the traditional discriminator in a GAN with an **invariance checker**.
- We consider **volume fraction** (p_1) and **two-point correlation** (p_2) as **invariances**.

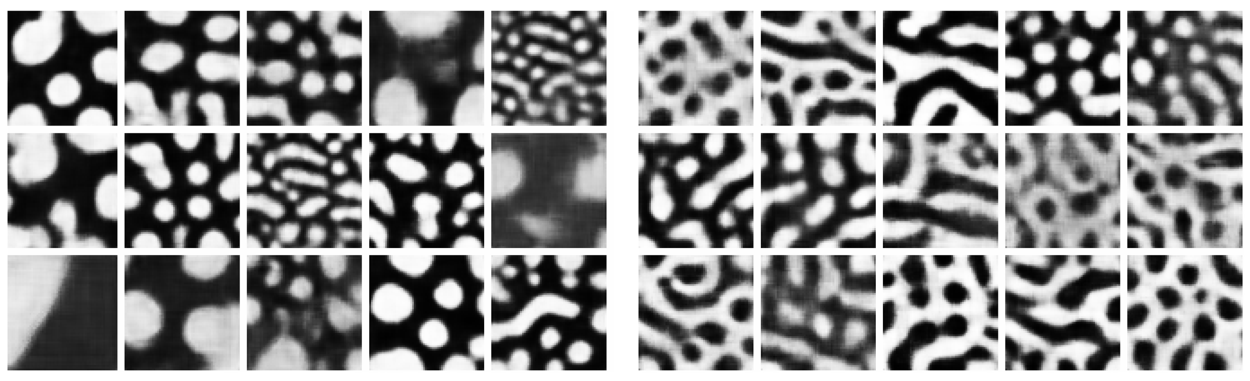
Wasserstein GAN with Gradient Penalty (WGAN-GP) [1]



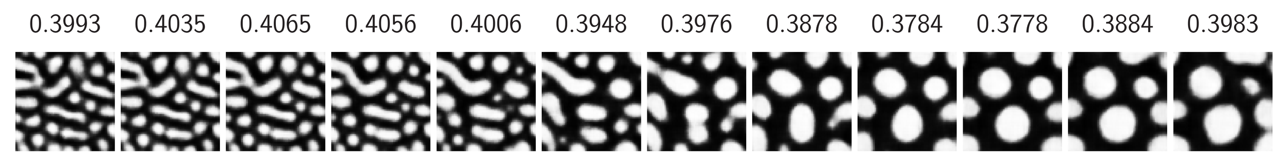
$$L = \underbrace{\mathop{\mathbb{E}}_{\tilde{\mathbf{x}}\sim\mathbb{P}_g}[D(\tilde{\mathbf{x}})] - \mathop{\mathbb{E}}_{\mathbf{x}\sim\mathbb{P}_r}[D(\mathbf{x})]}_{\text{Wasserstein loss}} + \underbrace{\lambda \mathop{\mathbb{E}}_{\hat{\mathbf{x}}\sim\mathbb{P}_{\hat{\mathbf{x}}}}\left[(\|\nabla_{\hat{\mathbf{x}}} D(\hat{\mathbf{x}})\|_2 - 1)^2\right]}_{\text{Gradient penalty}}.$$



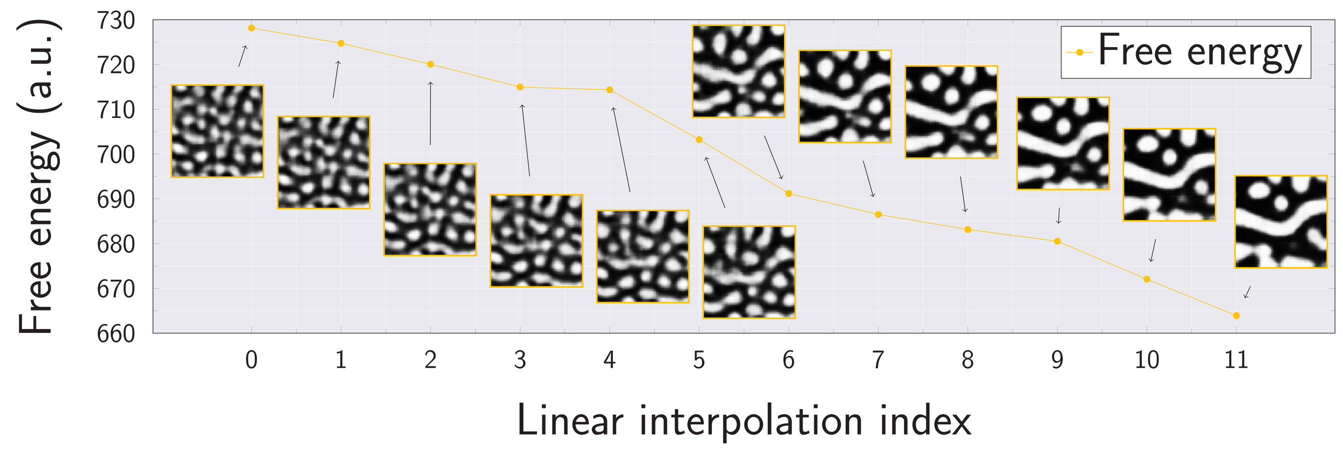
Training data(Cahn-Hilliard eqn.) Generated on CH dataset



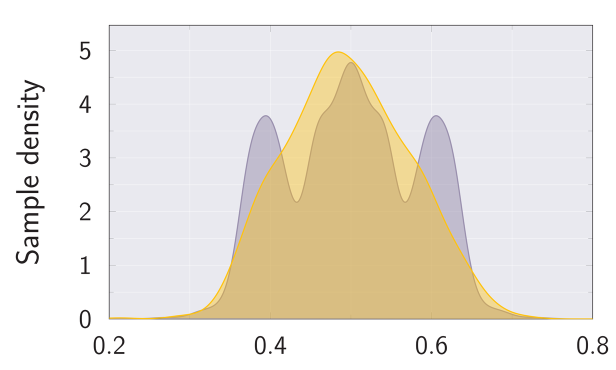
Generated on CH_{p1} dataset Generated on CH_{p2} dataset



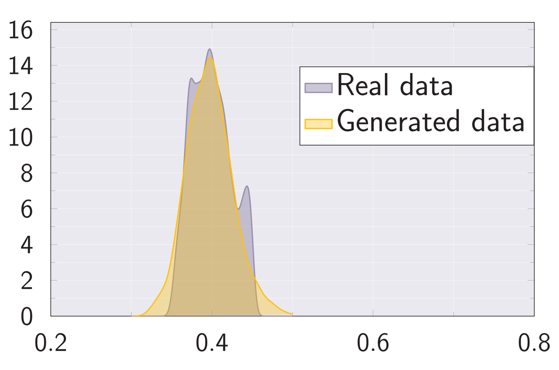
(a) Volume fraction is maintained in interpolation



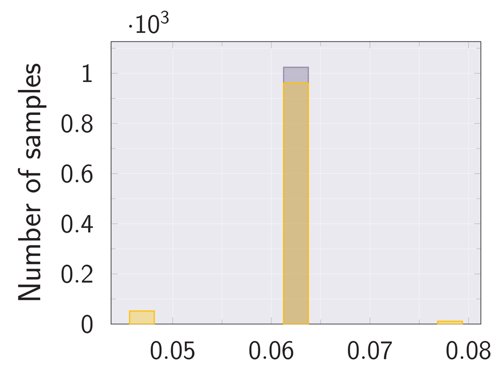
(b) We pick two morphologies with same volume fraction but with different free energies. The model can interpolate between these morphologies and produces realistic morphologies that exhibit a monotone energy behavior.



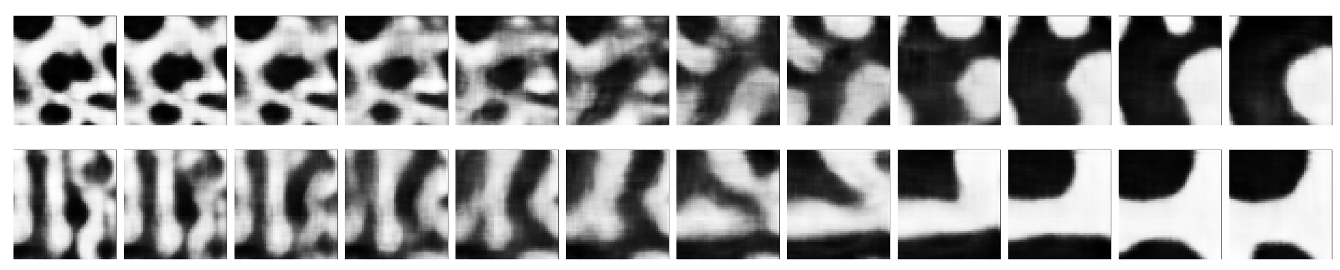
Volume fraction density plot for CH data



Volume fraction density plot for CH_{p1} data

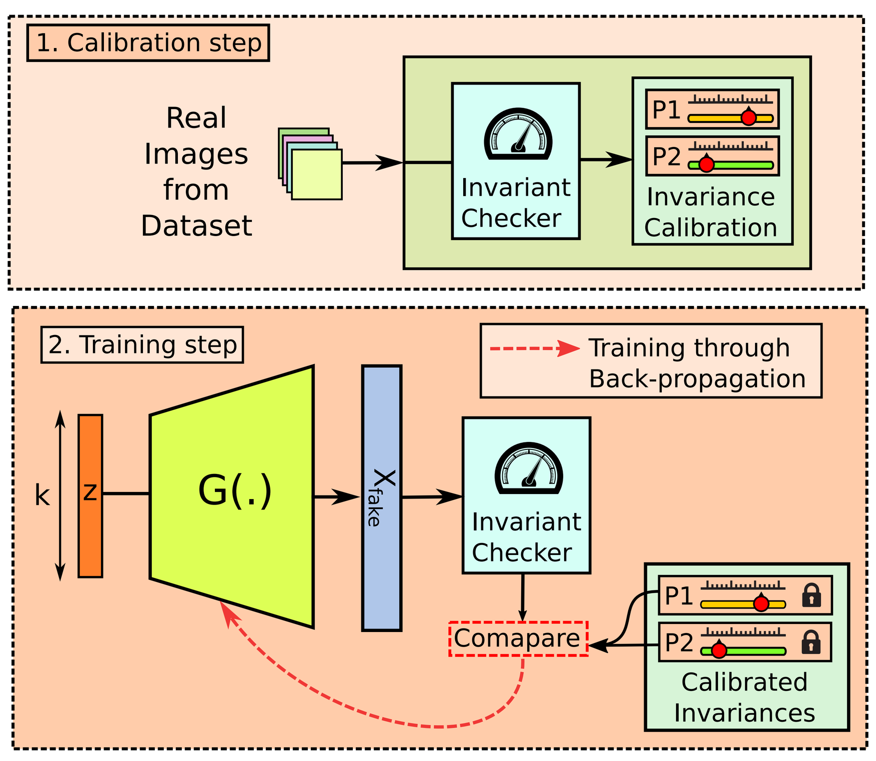


p_2 value

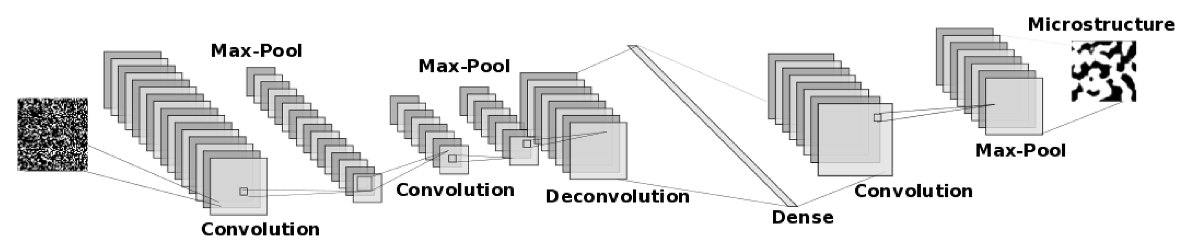


Results of the linear interpolation over latent variable z for WGAN-GP trained over the entire CH dataset.

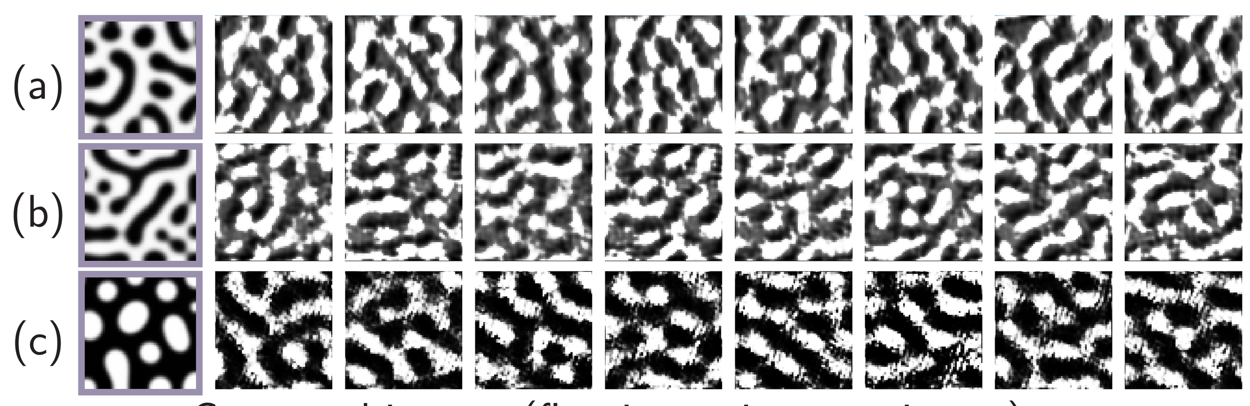
Generative Invariant Network (GIN)



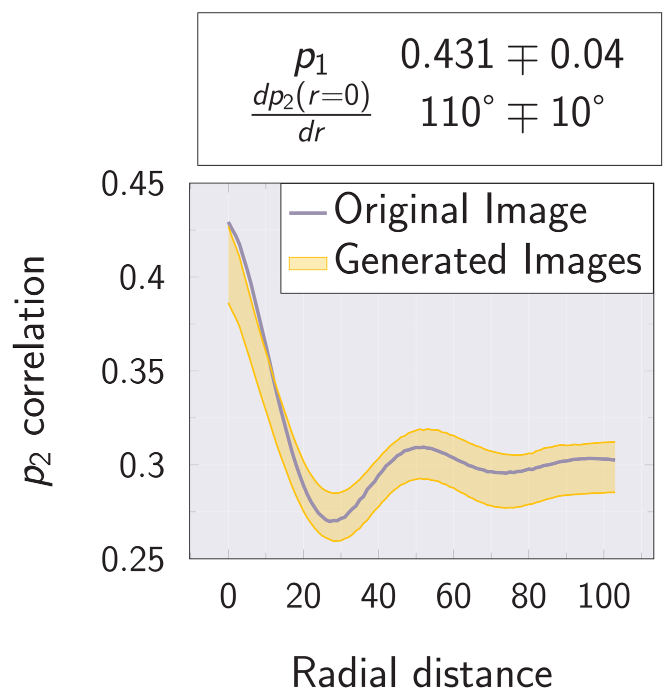
$$L_{inv} = \lambda_1 \sum_i |p_1^{(g)} - p_1^*| + \lambda_2 \sum_i \|p_2^{(g)} - p_2^*\|_2, \quad g \in \mathcal{G}.$$



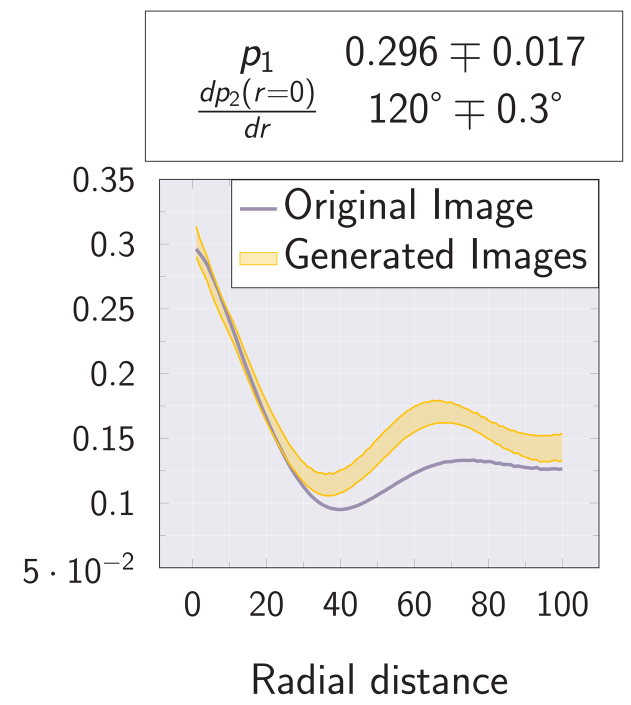
Generator architecture for GIN



Generated images (first image is target image)

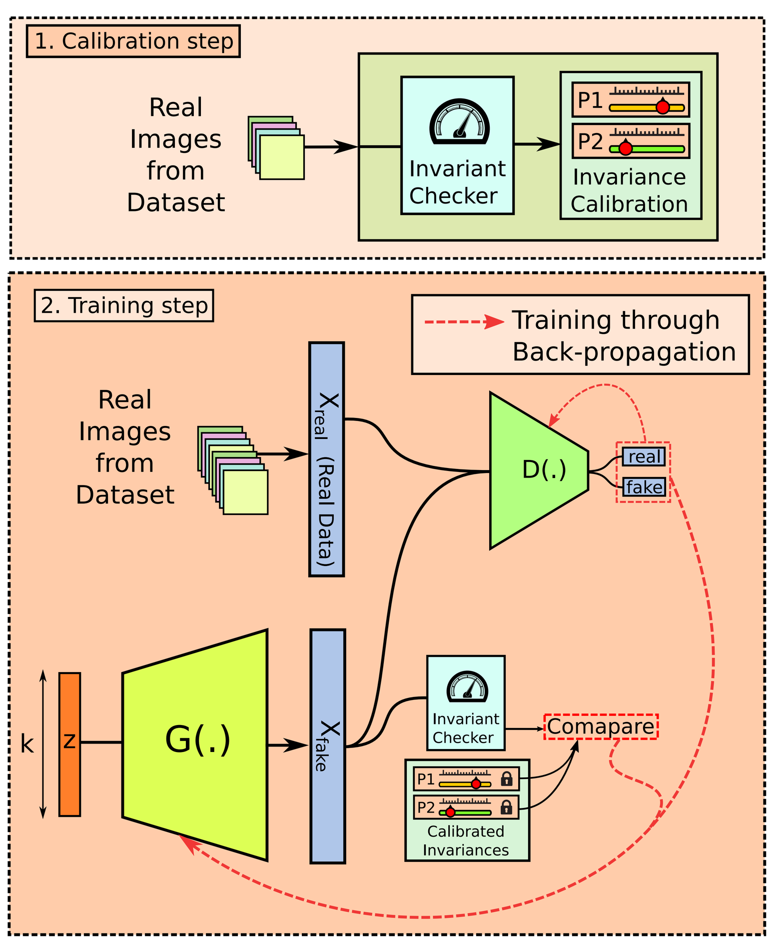


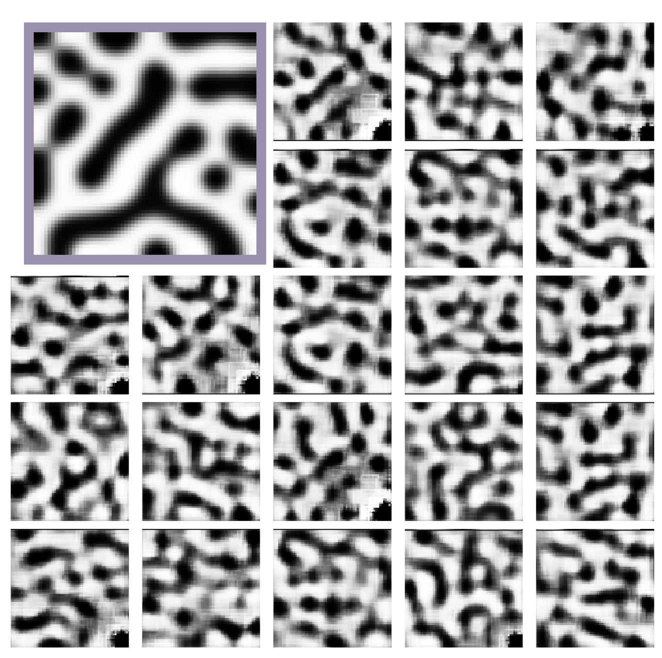
(a) GIN trained on entire p_2 curve



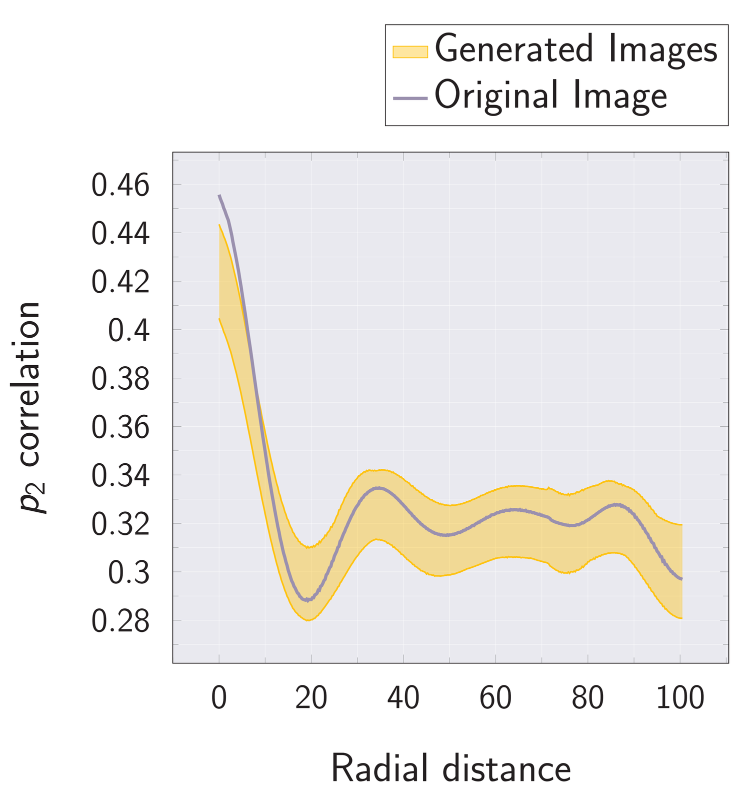
(b) GIN trained on initial p_2 curve

Hybrid (GAN+GIN) Model

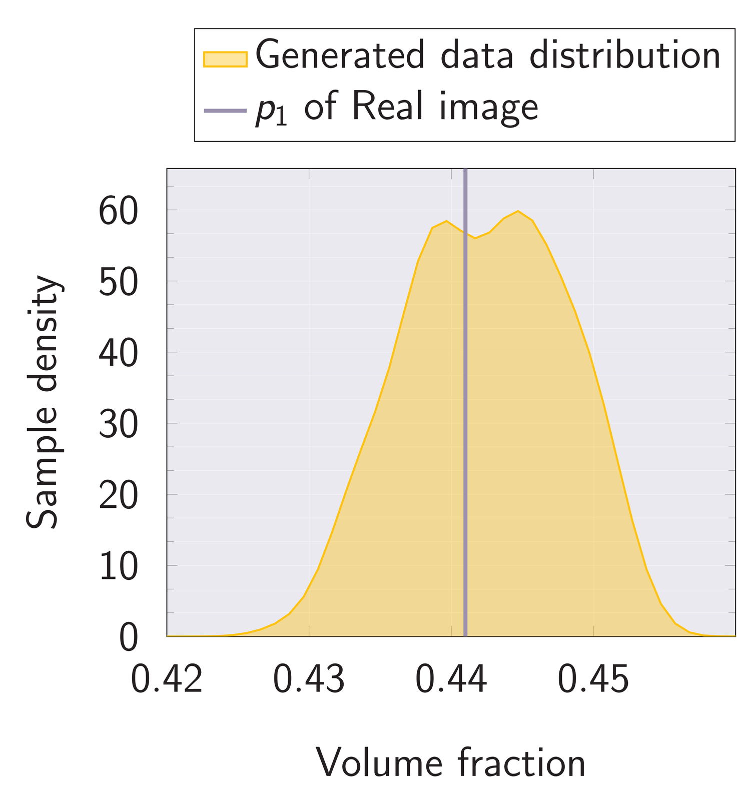




(a) Generated images (target image on top left)



(b) 2−point correlation curves



(c) Distribution of p_1

References

[1] Gulrajani, I., Ahmed, F., Arjovsky, M., Dumoulin, V. and Courville, A.C., 2017. Improved training of Wasserstein gans. NeurIPS.

[2] Adams, B.L., Kalidindi, S. and Fullwood, D.T., 2012. Microstructure sensitive design for performance optimization. Butterworth-Heinemann.

[3] Materials Genome Initiative. url: https://www.mgi.gov/.

[4] Singh, R., Shah, V., Pokuri, B., Sarkar, S., Ganapathysubramanian, B., Hegde, C., 2018. Physics-aware Deep Generative Models for Creating Synthetic Microstructures. NeurIPS MLMM Workshop. **arXiv:1811.09669. url: https://arxiv.org/abs/1811.09669**.