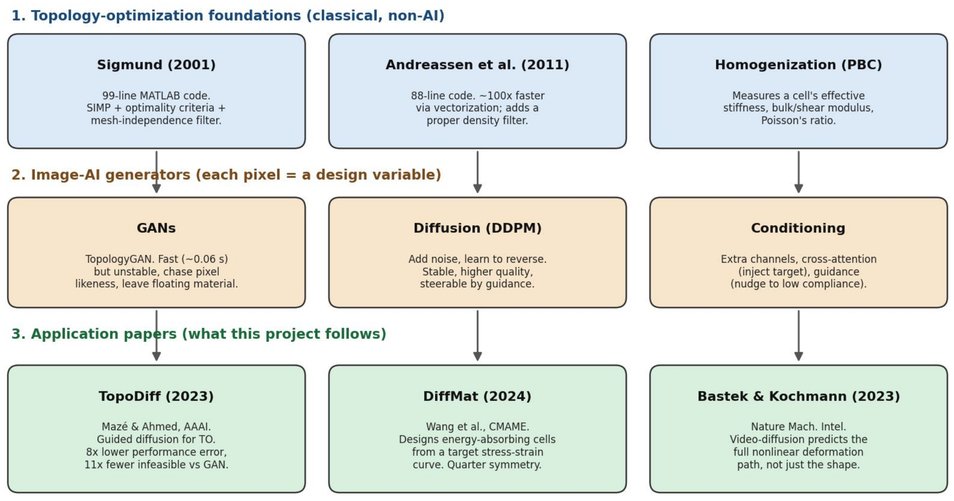
Generative AI for Designing Topology-Optimized Metamaterial Unit Cells

1. Background

- A metamaterial gets its behavior from geometry, not material. The same plastic, arranged differently, can be stiff, soft, or expand sideways when stretched (auxetic).
- A 2D unit cell is a binary image: white = solid, black = void. Tiling the small cell builds the material.
- Topology optimization finds efficient layouts; recent work generates them with AI.

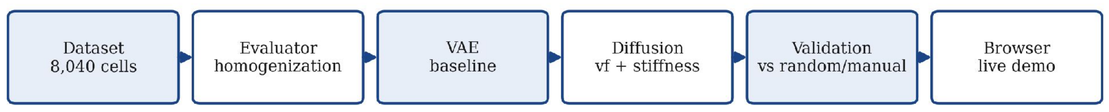


This project = Sigmund/Andreassen-style data + small conditional diffusion + homogenization evaluation

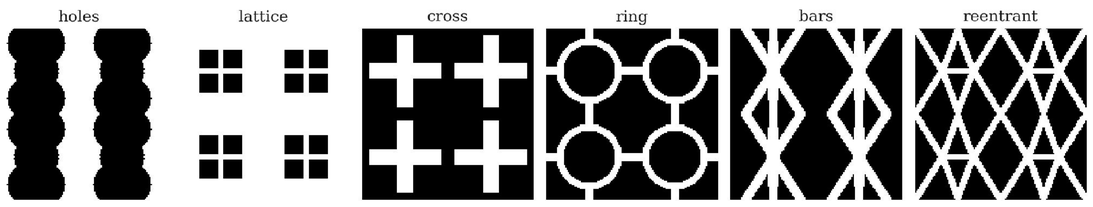
2. Objective

Research question: Can a generative AI model learn from topology-like designs and produce new unit cells with useful, targeted mechanical behavior, such as a chosen volume fraction and stiffness?

3. Methods: Pipeline



4. Dataset



- 8,040 binary 64×64 cells across six families.
- Each labeled with volume fraction and homogenized stiffness.
- A synthetic stand-in for real topology-optimization output.

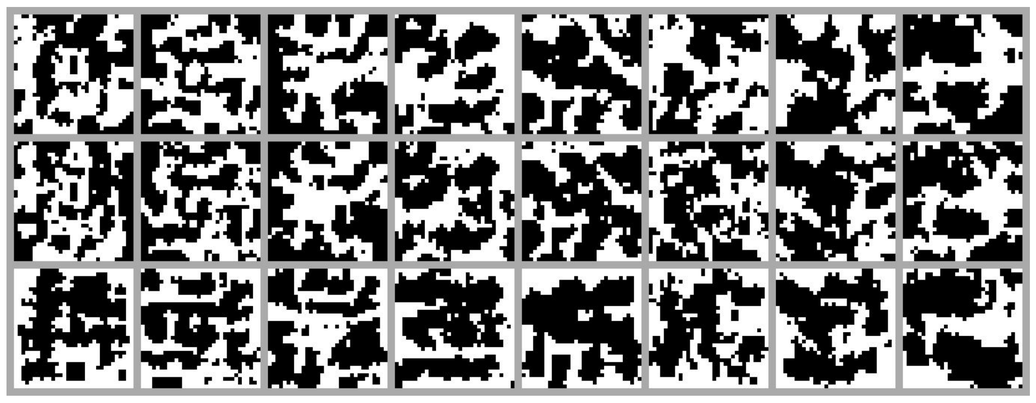
5. Mechanical Analysis

- Periodic homogenization returns effective stiffness, Poisson's ratio, and connectivity.
- Validated against known cases before use:

Test case	Expected	Result
Solid cell	$E = 1.0$, $\nu = 0.30$	matched
Layered cell	Voigt / Reuss bounds	matched
Auxetic base $\nu = -0.3$	recovered exactly	matched

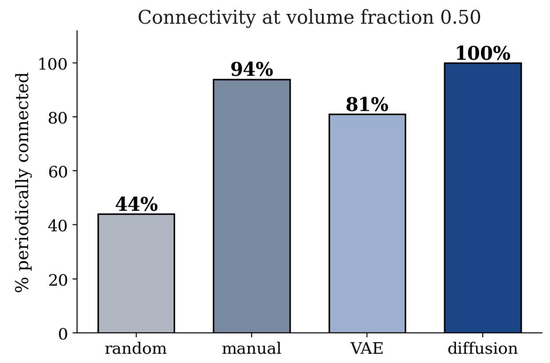
6. Generative Models

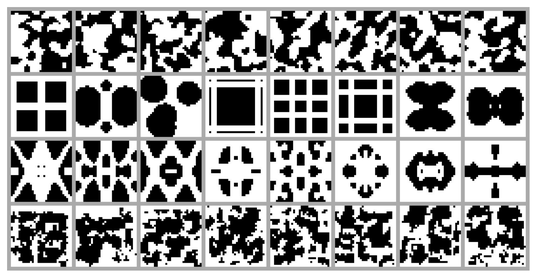
- Baseline: conditional VAE. Reconstructs well (IoU 0.98) but fragments at low density.
- Diffusion: small conditional DDPM, conditioned on volume fraction and stiffness class, with EMA.
- Checkpoint chosen by controllability, not by loss.



Diffusion samples conditioned low / medium / high stiffness (top to bottom).

7. Results





Source (vf 0.50)	vf err	connected	E_eff
random	0.00	44%	0.013
manual	0.024	94%	0.274
VAE	0.138	81%	0.246
diffusion	0.013	100%	0.095

- Diffusion hits the target volume fraction within 0.02 and is 100% connected; it beats random on every structural metric.
- Stiffness separates about 2× between the low and high classes.
- Manual designs still reach the highest absolute stiffness; the VAE only looks stiff because it overshoots density (vf error 0.14).

8. Conclusion & Future Work

- Yes: generative models produce candidates categorically better than random, connected versus fragmented, stiff versus limp, and steerable to a requested property.
- Honest limits: synthetic data; volume-fraction control compressed to ~0.37–0.57; no auxetic cells; speckly outputs.
- Next: train on real topology-optimized data, and add guidance to the diffusion sampler instead of filtering afterward.