

# The Development of an NETL DAC Reactor: Optimization of Direct Air Capture (DAC) Reactor Configuration Using Artificial Intelligence (AI) Inverse Engineering Techniques

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## Goal

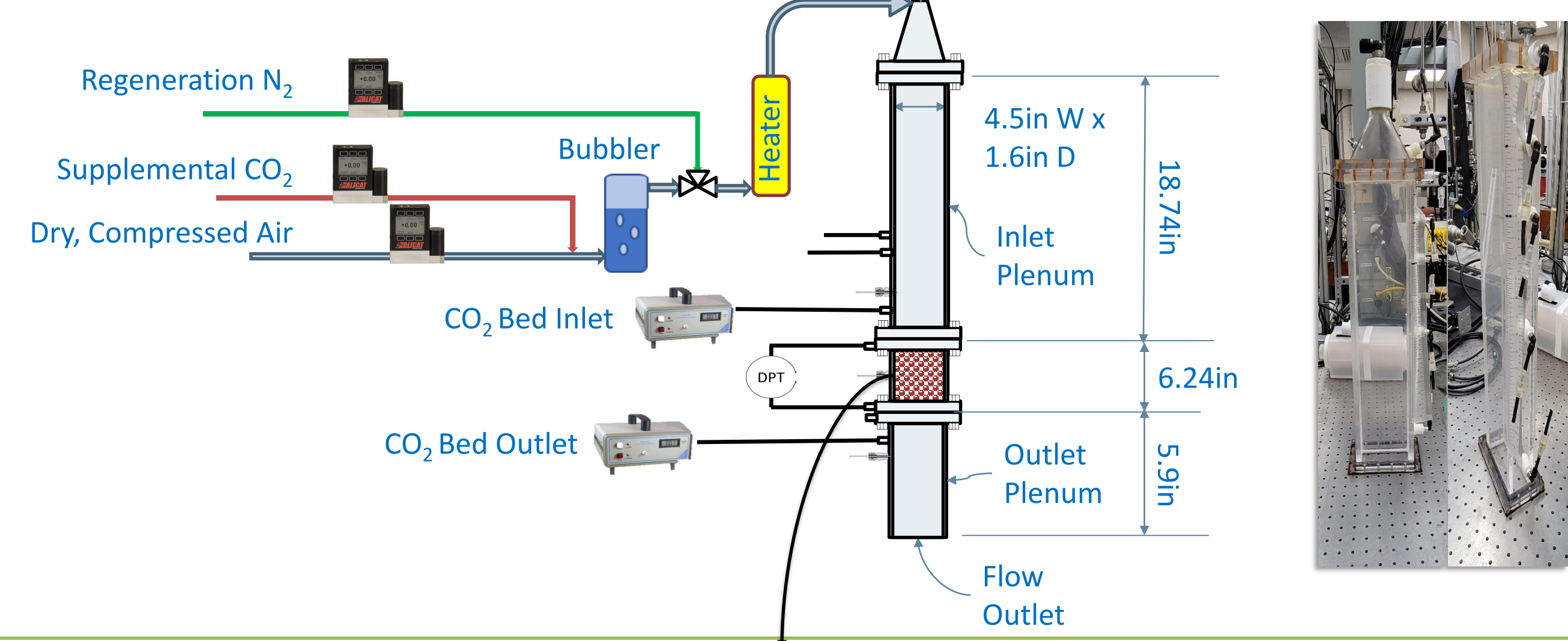
Use generative design techniques to optimize direct air capture (DAC) material packing configurations. Fan power requirements are a significant operation cost, can we use innovative structures to reduce pressure drop while maintaining capture rates?

**Objective**

$$\max \frac{CO_{2,in} - CO_{2,out}}{CO_{2,in}} * 100$$

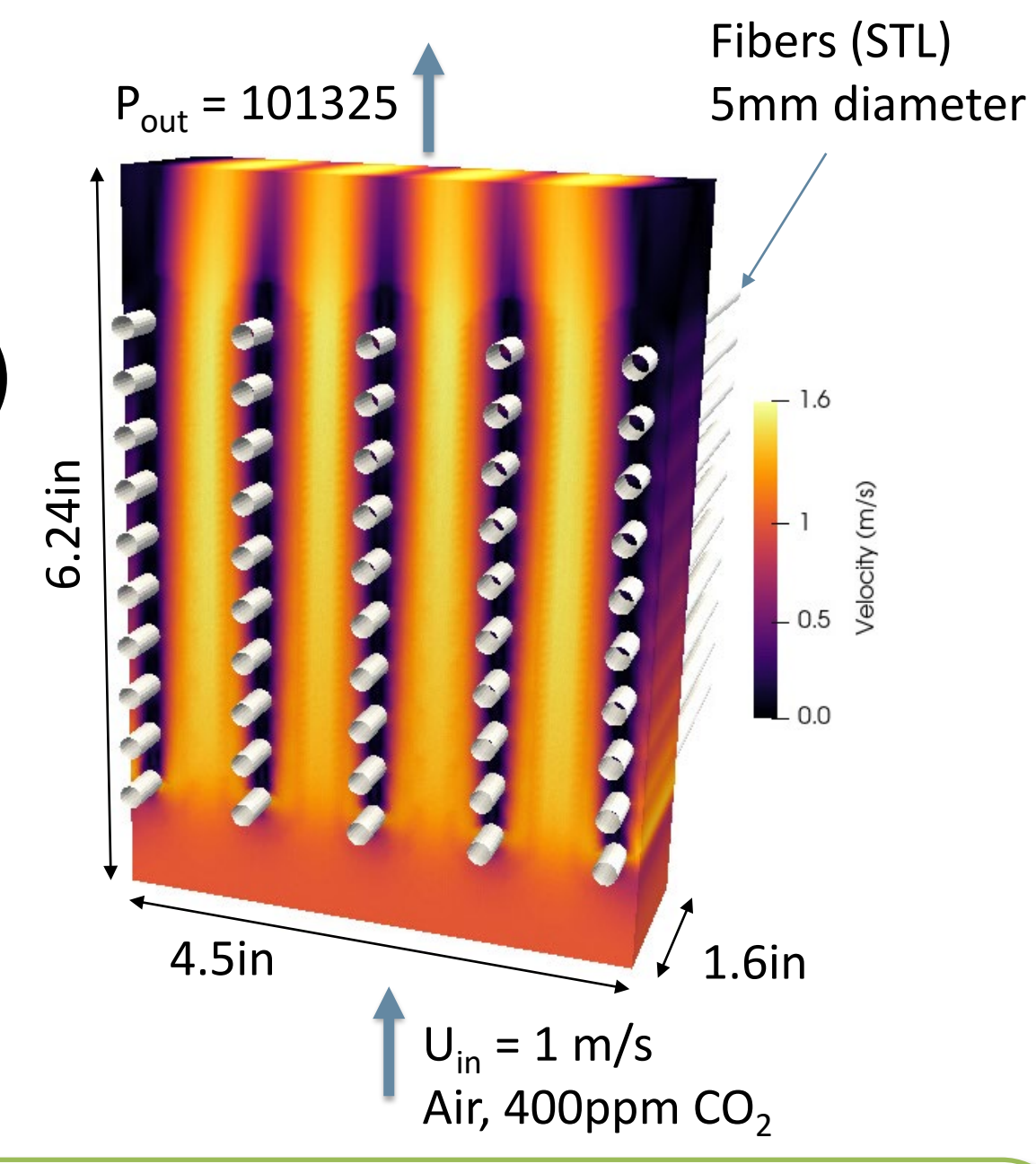
$$\frac{\Delta P}{\Delta P}$$

## Experiment

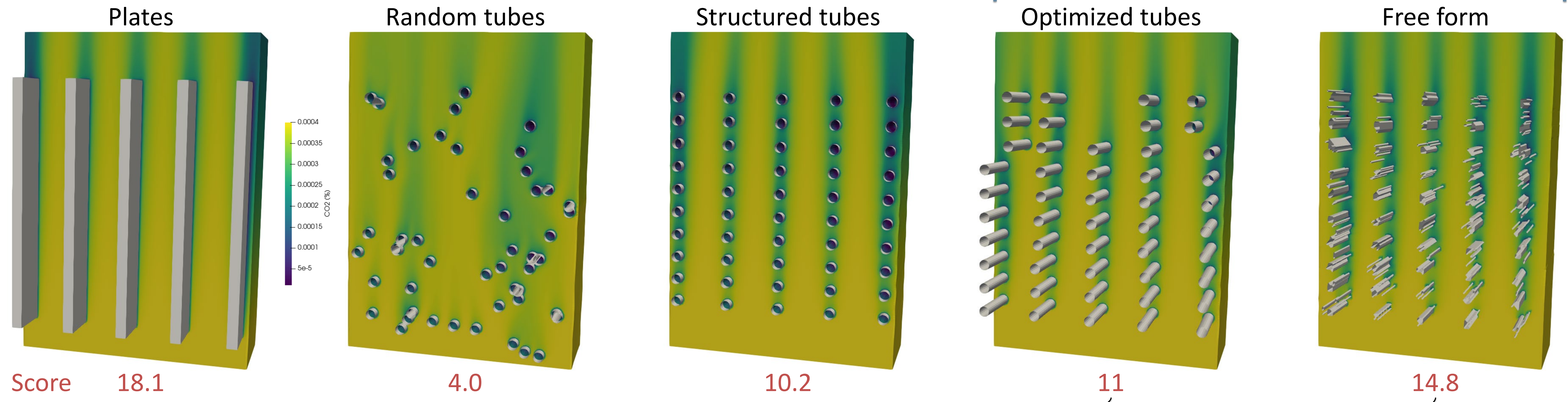


## CFD model

**Solver:** simpleFoam (steady state)  
**Mesh:** 210k cells  
**Turbulence:** kOmegaSST  
**Runtime:** 4 Cores, meshes in 20s, runs in 3.5 minutes

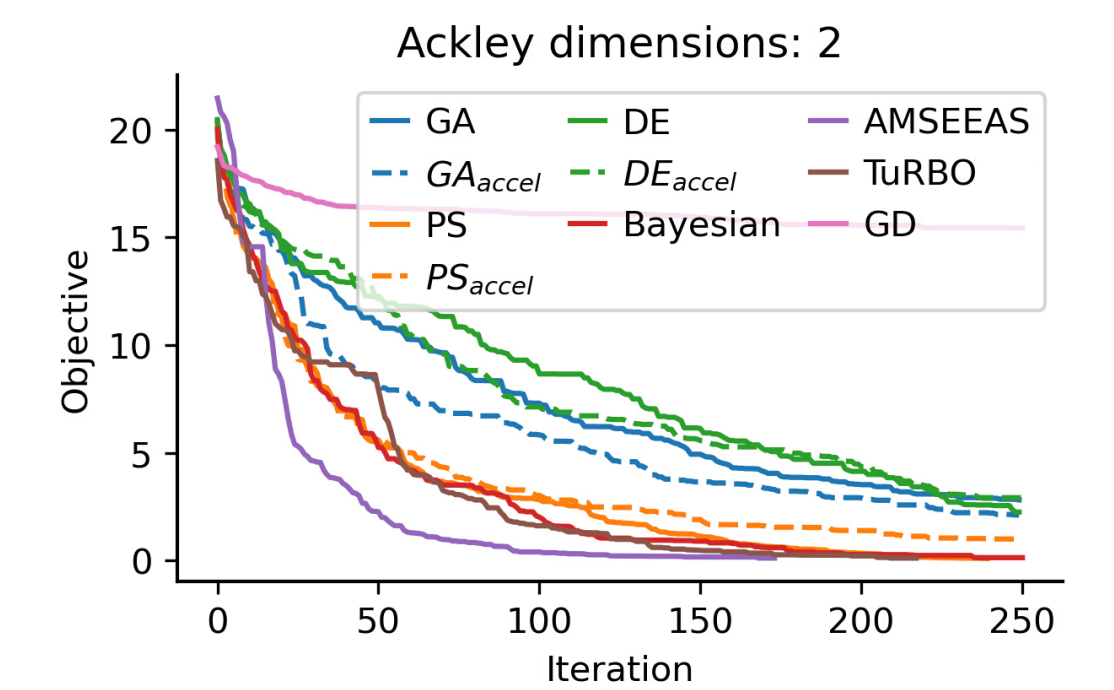


## What's the best configuration?

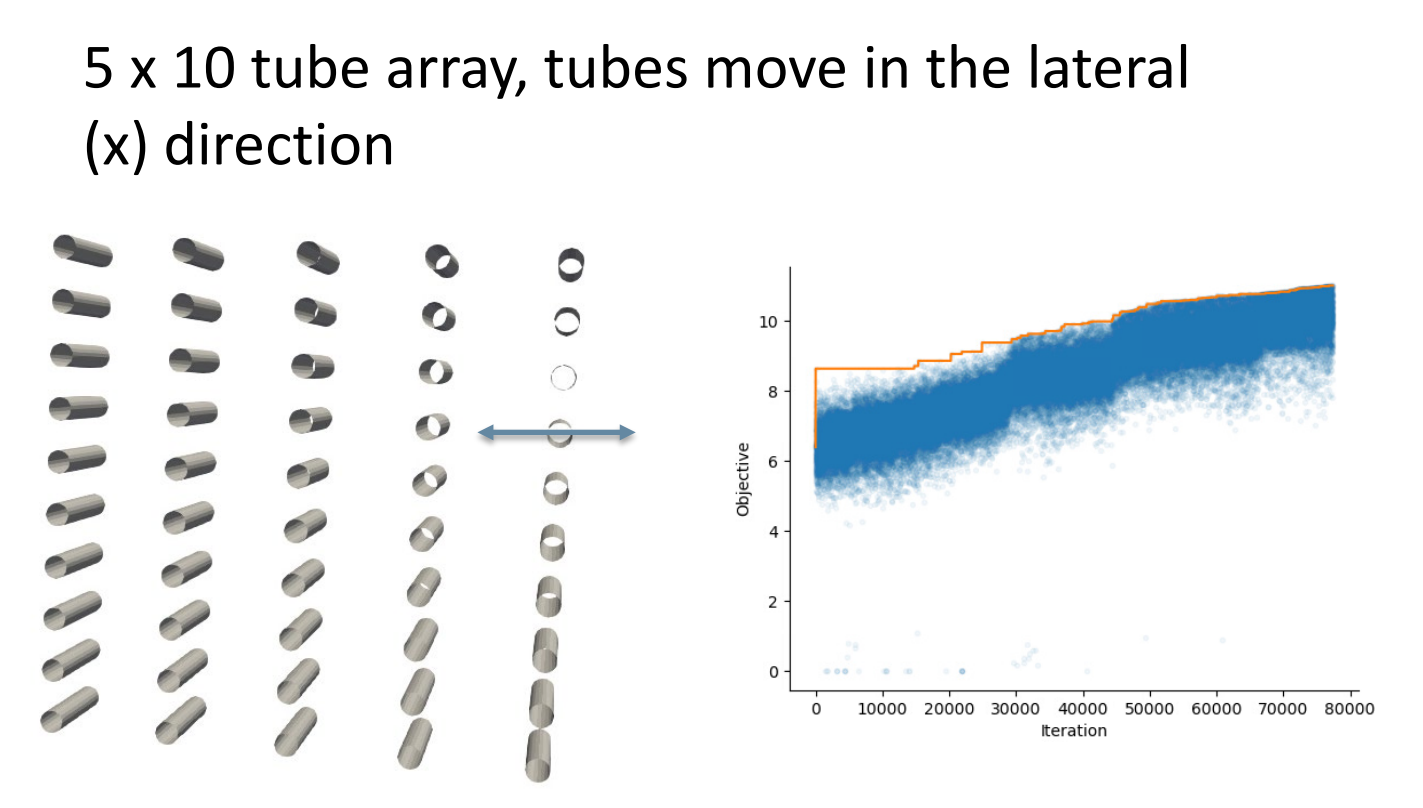


## Algorithms

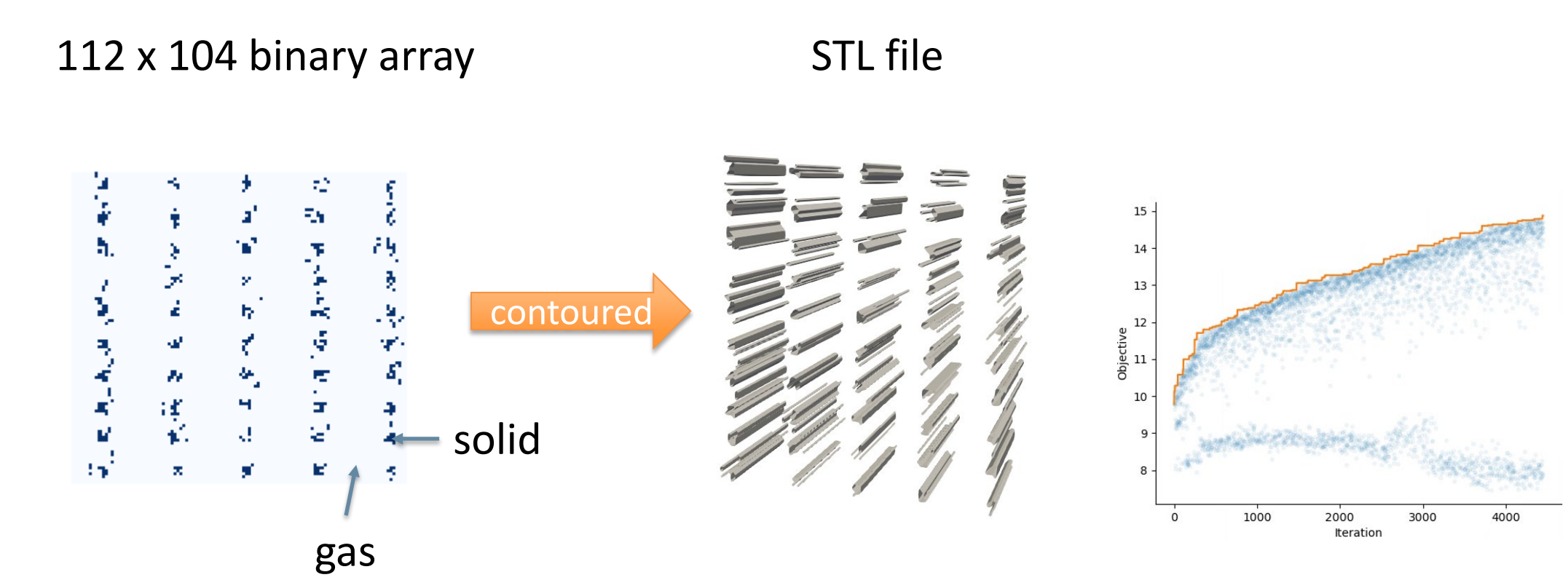
- Genetic algorithm (GA)
- Particle swarm (PS)
- Differential evolution (DE)
- Bayesian optimization
- TURBO
- AMSEES
- Gradient Descent (GD)



## GA with lateral spacing



## GA with binary level set



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