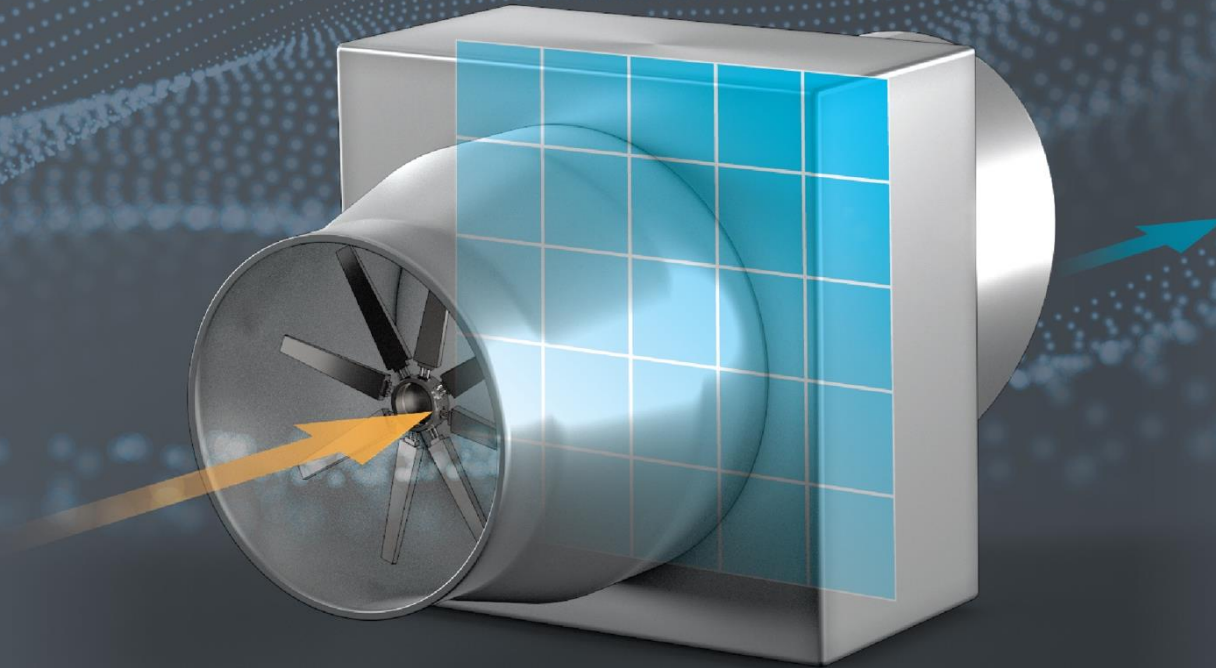


The Development of an NETL DAC Reactor: Optimization of Direct Air Capture (DAC) Reactor Configuration Using Artificial Intelligence (AI) Inverse Engineering Techniques

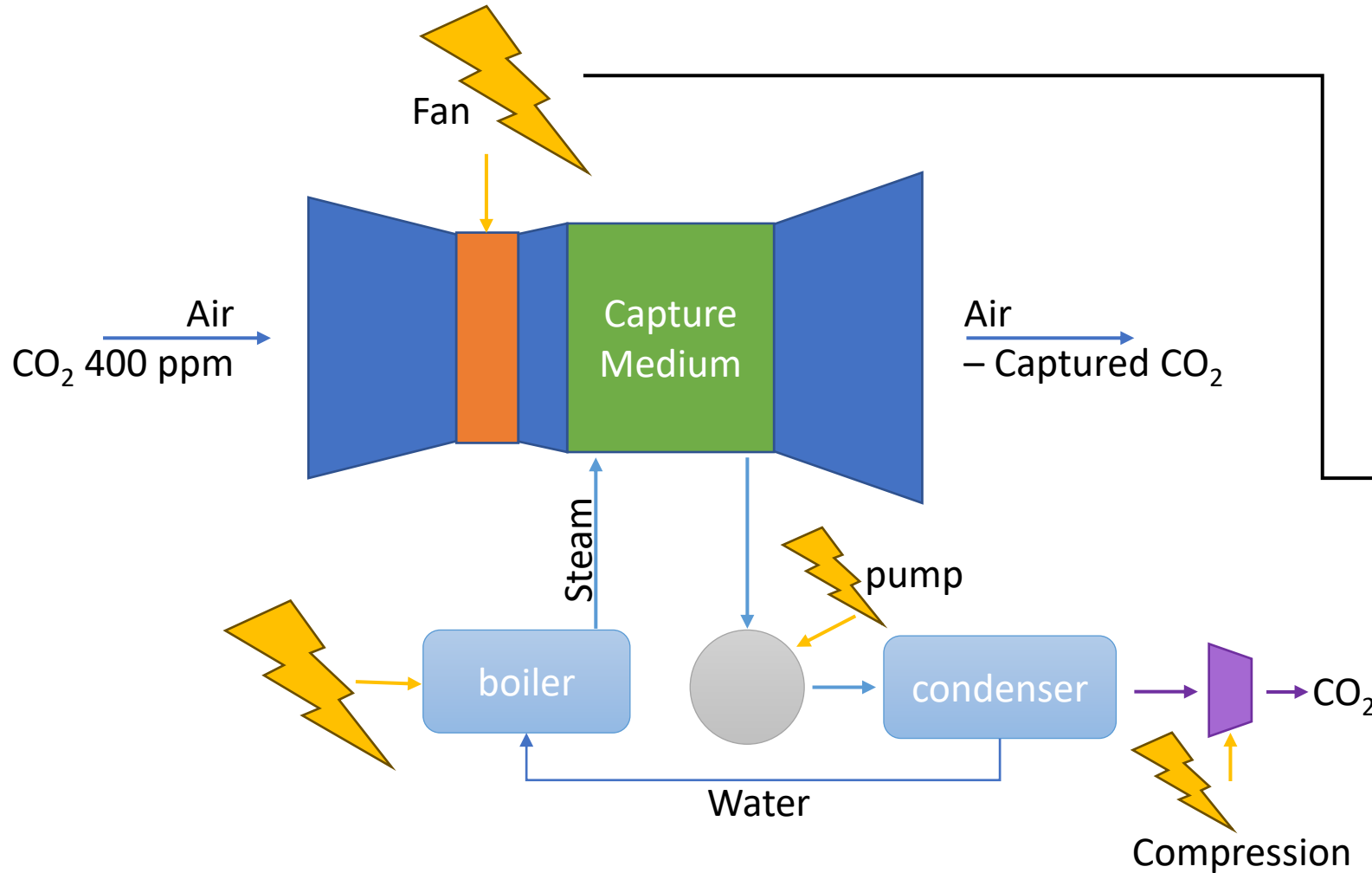


Justin Weber, Jarrett Riley, Steven Rowan, Ronald Breault



Tuesday , August 29, 2023

Challenge: Reduce the cost of DAC



CASE 0B-EB – ELECTRIC BOILER

Performance Summary	
Total Gross Power, MWe	0
DAC Air Fans, kWe	28,800
DAC CO ₂ Compression, kWe	1,490
Electric Boiler, kWe	19,510
Balance of Plant, kWe	163
Total Auxiliaries, MWe	50
Net Power, MWe	-50
DAC CO ₂ Removed from Air (Gross), tonnes/yr	100,000
Net CO₂ Removed from Air, tonnes/yr	100,000

J. Valentine, A. Zoelle, "Direct Air Capture Case Studies: Sorbent System," National Energy Technology Laboratory, Pittsburgh, PA, July 8, 2022.

Polymers with intrinsic microporosity (PIMs)

What is the best form factor?

plates



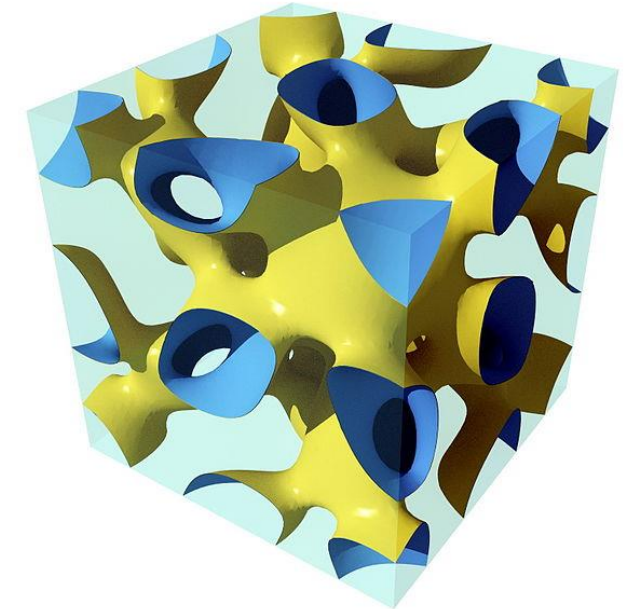
tubes



Mat/felt



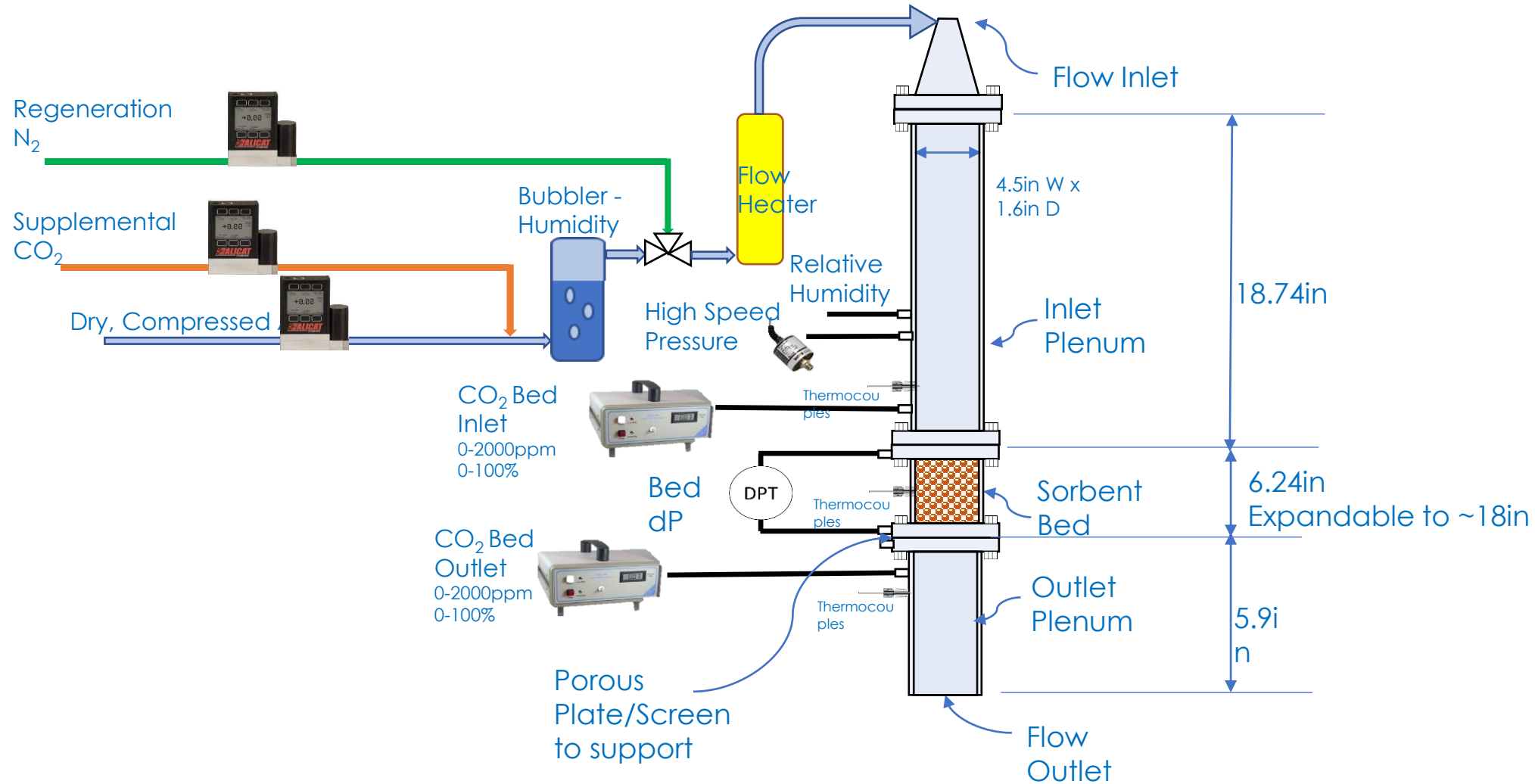
Gyroids



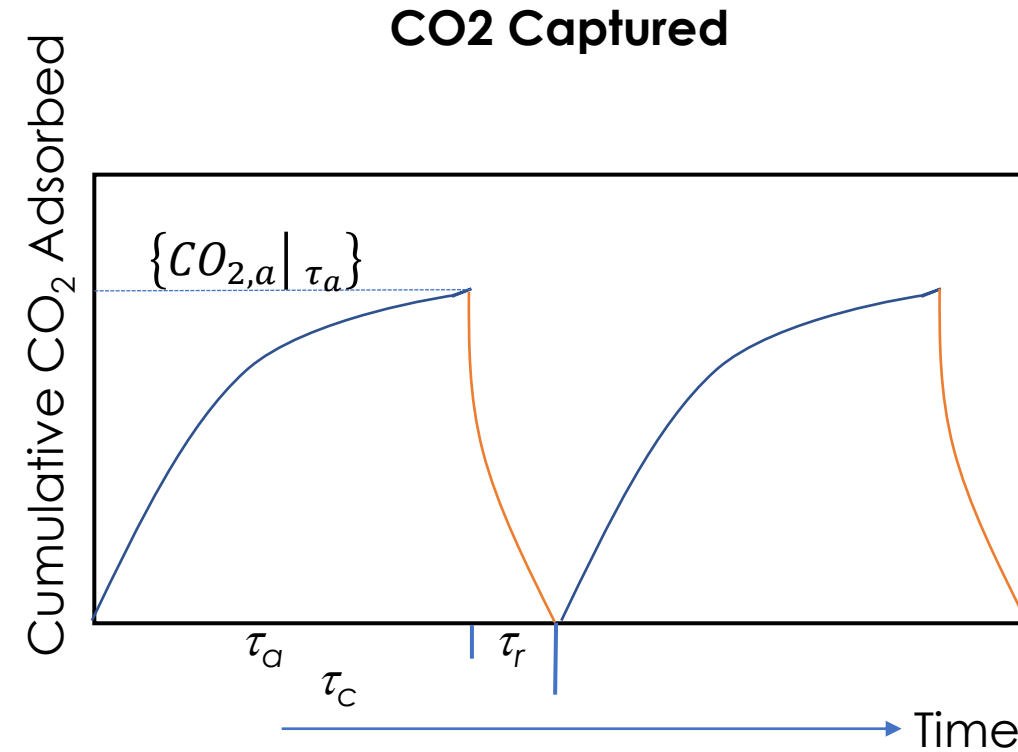
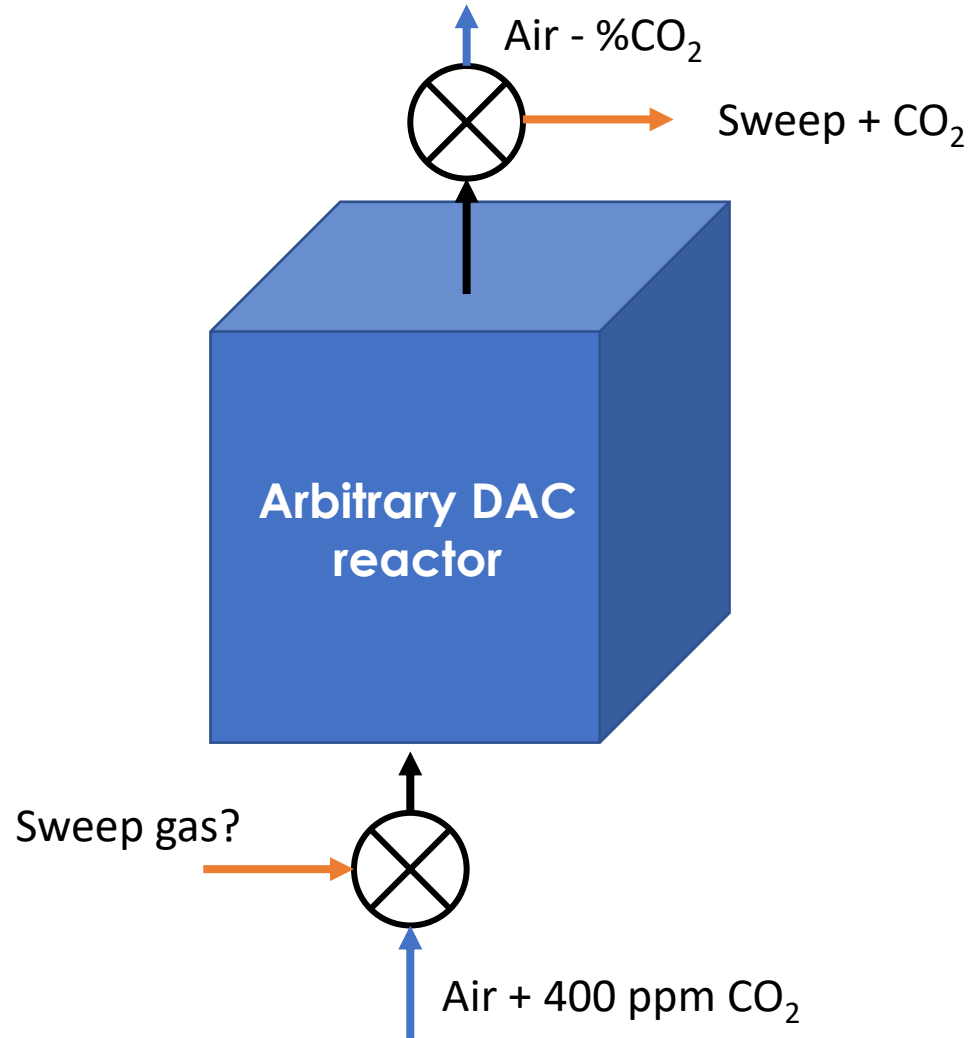
Objective: Maximize: Mass transfer
Minimize: Pressure drop

Anders Sandberg,
https://commons.wikimedia.org/wiki/File:Lidinoid_surface.jpg

Lab scale test unit



DAC process



$$CO_{2,D} = \{CO_{2,a} | \tau_a\} N_{cycles}$$

Generative design (optimization)

Use AI algorithms with computational models to generate and evaluate multiple design alternatives

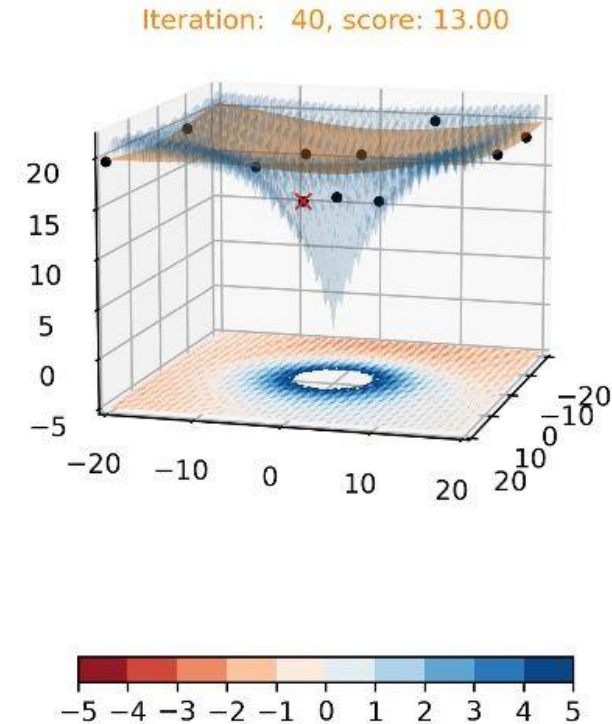
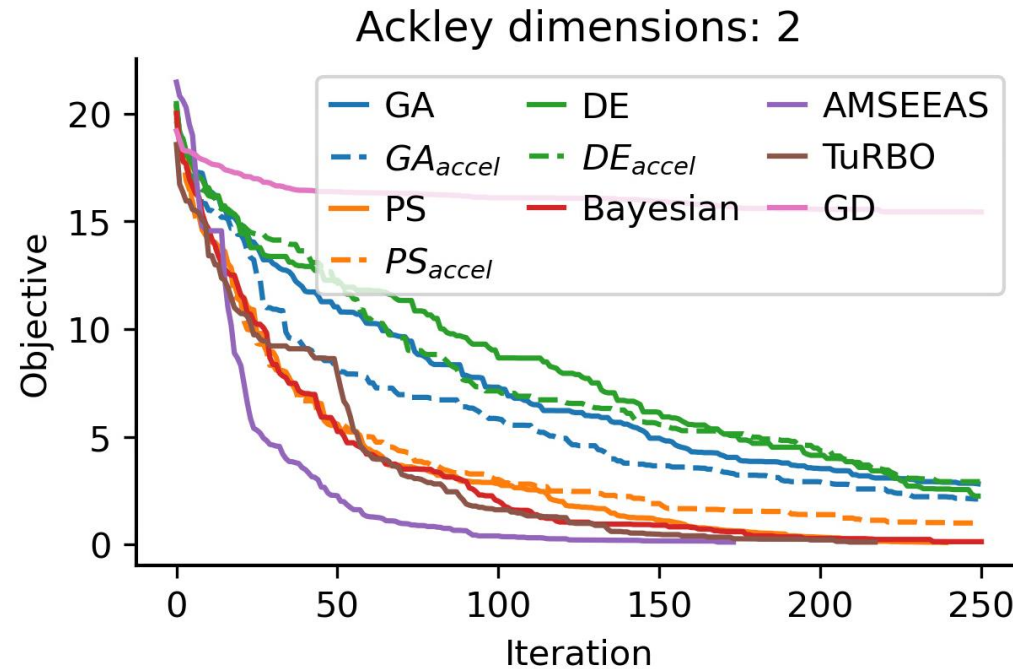
Genetic algorithm (GA)
Particle swarm (PS)
Differential evolution (DE)
Bayesian optimization
TuRBO
AMSEEAS
Gradient Descent (GD)



Meta model accelerator



Minimize the
number of expensive
function calls



Generative design (optimization)

Use AI algorithms with computational models to generate and evaluate multiple design alternatives

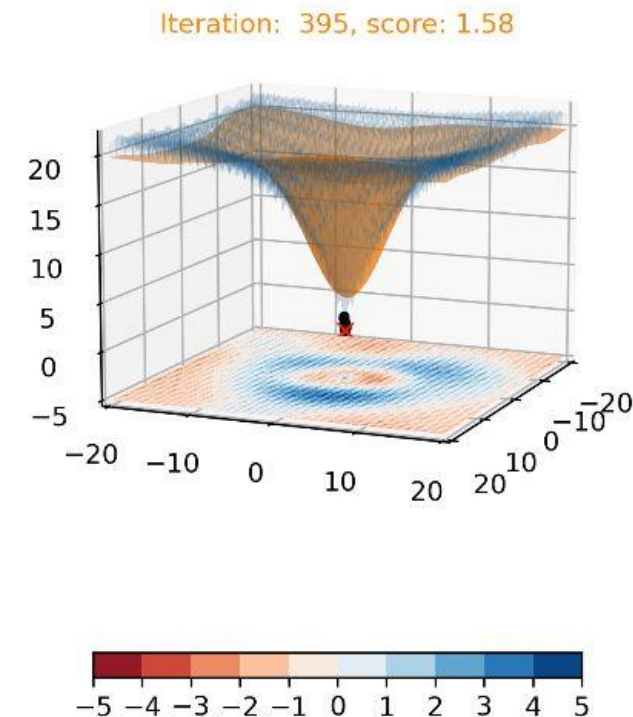
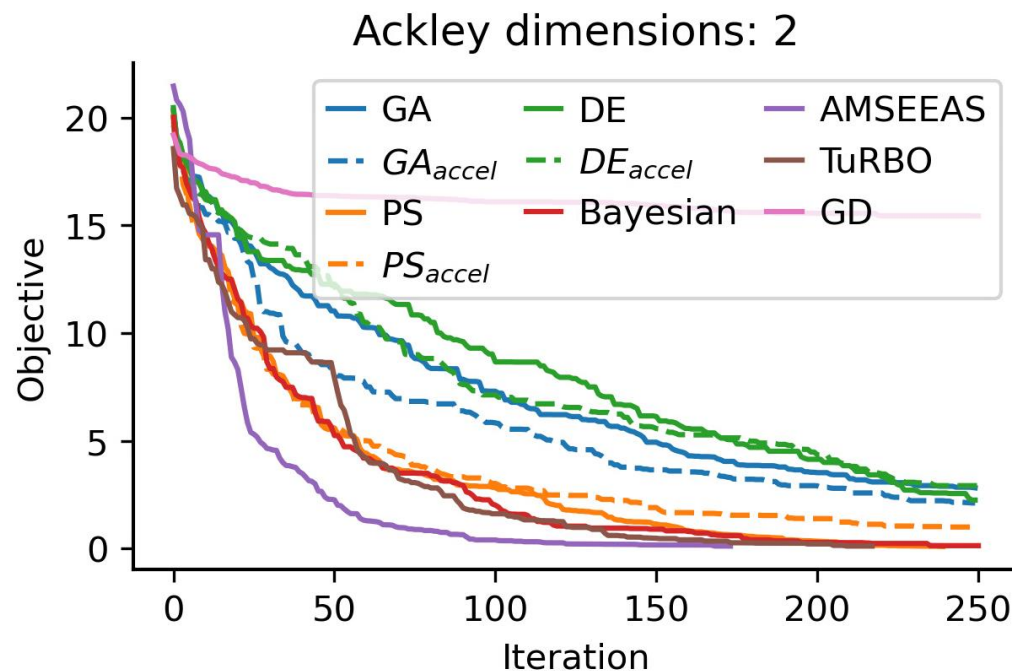
Genetic algorithm (GA)
Particle swarm (PS)
Differential evolution (DE)
Bayesian optimization
TuRBO
AMSEEAS
Gradient Descent (GD)



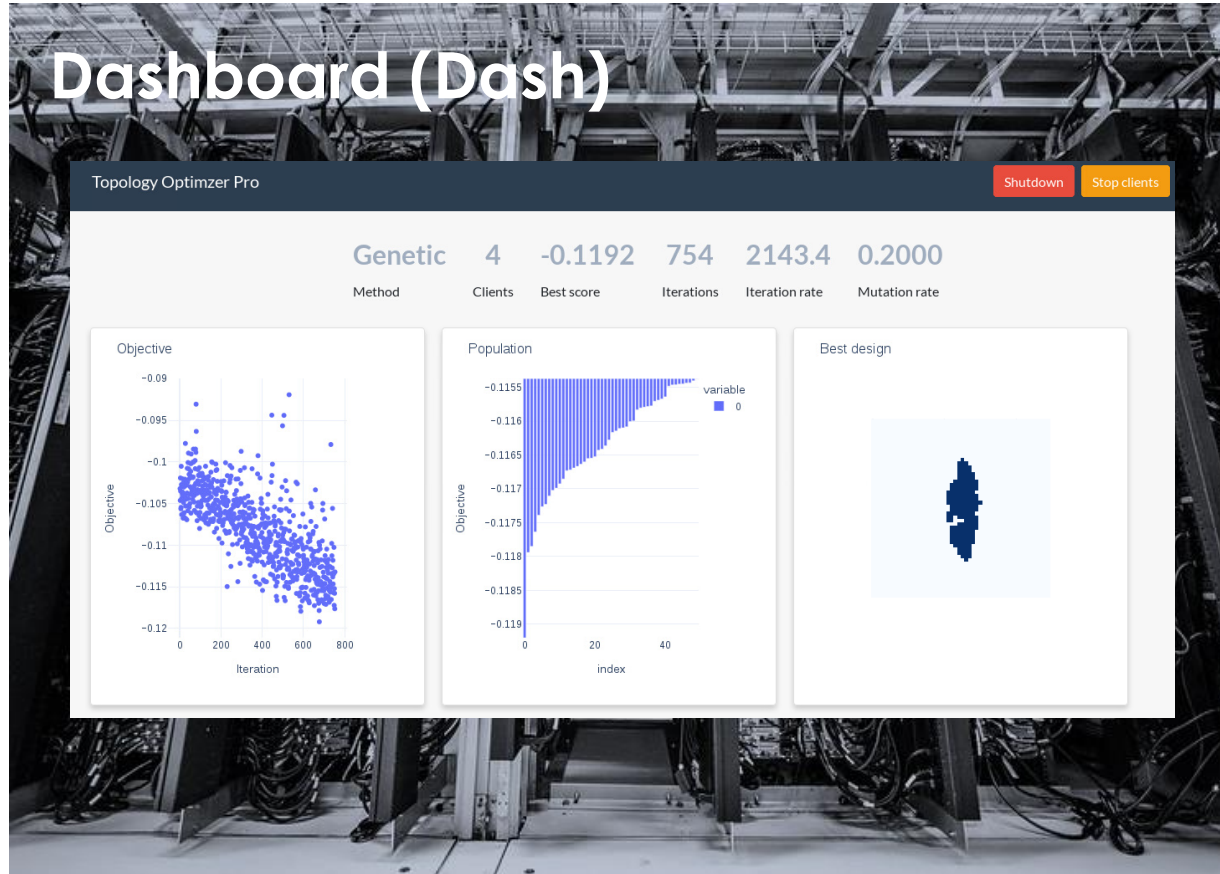
Meta model accelerator



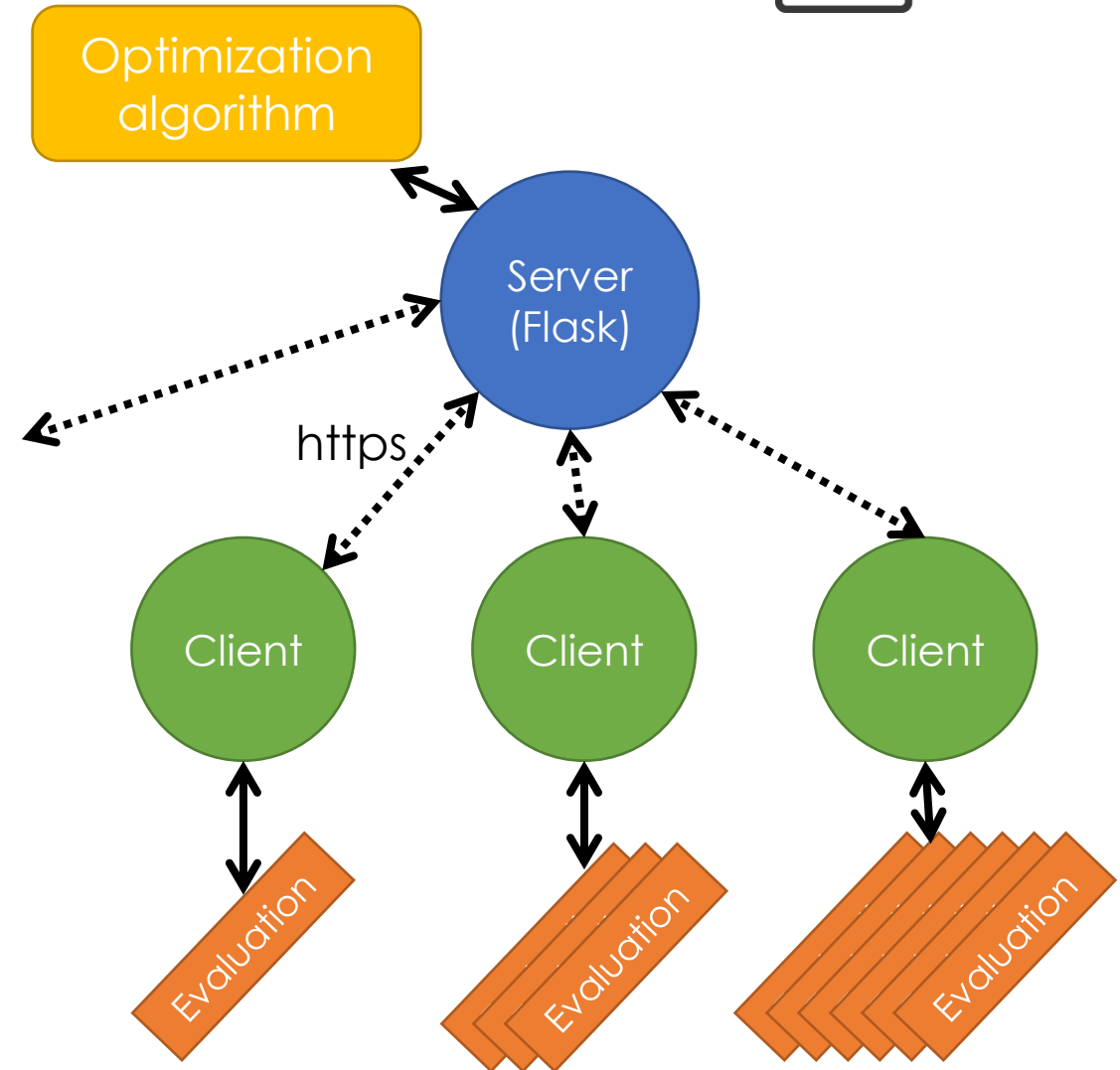
Minimize the
number of expensive
function calls



Custom framework for large scale campaigns



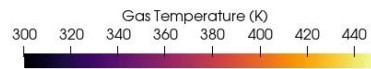
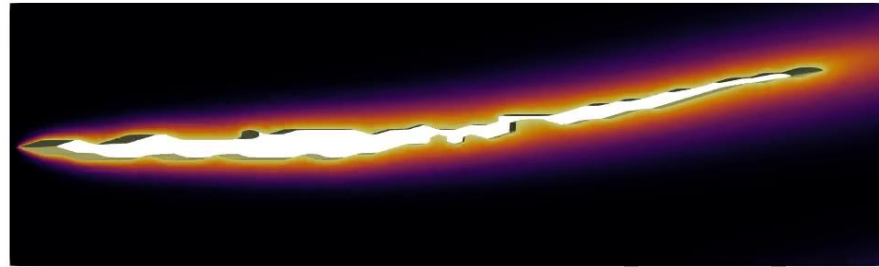
- Allows for distributed computing
- Thousands of simultaneous evaluations



Example usage: Aerothermal/heat transfer

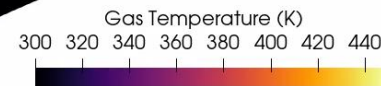
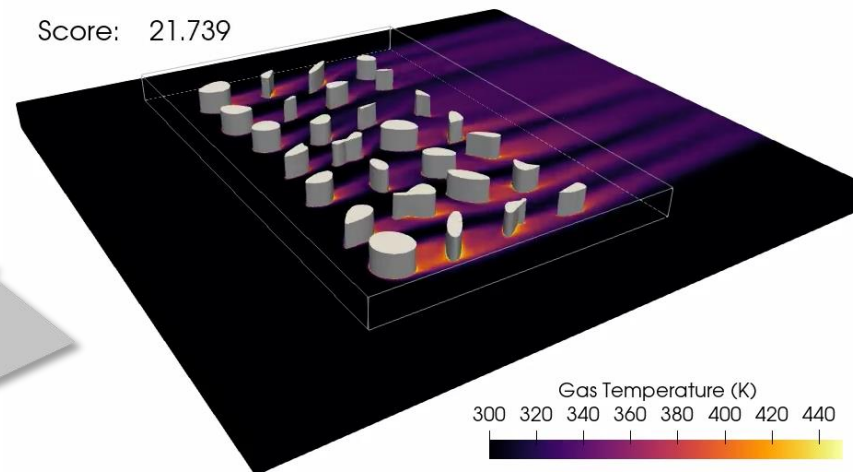
Single pin fin

Score: -0.135



Pin fin array

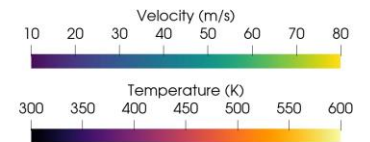
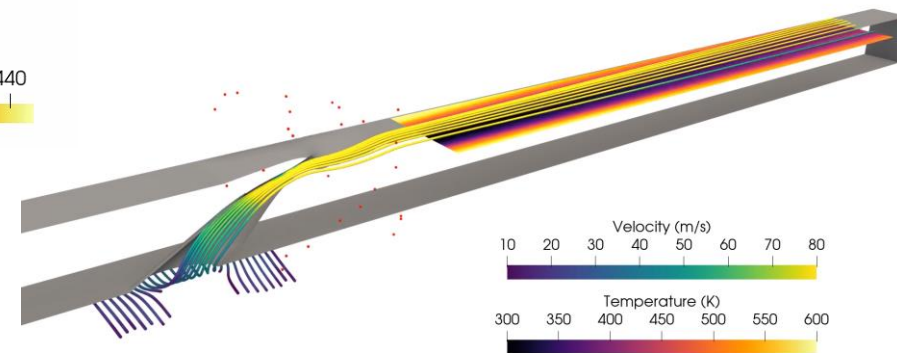
Score: 21.739



$7 \times 4 \times 4 \times 2 = 224$ dims

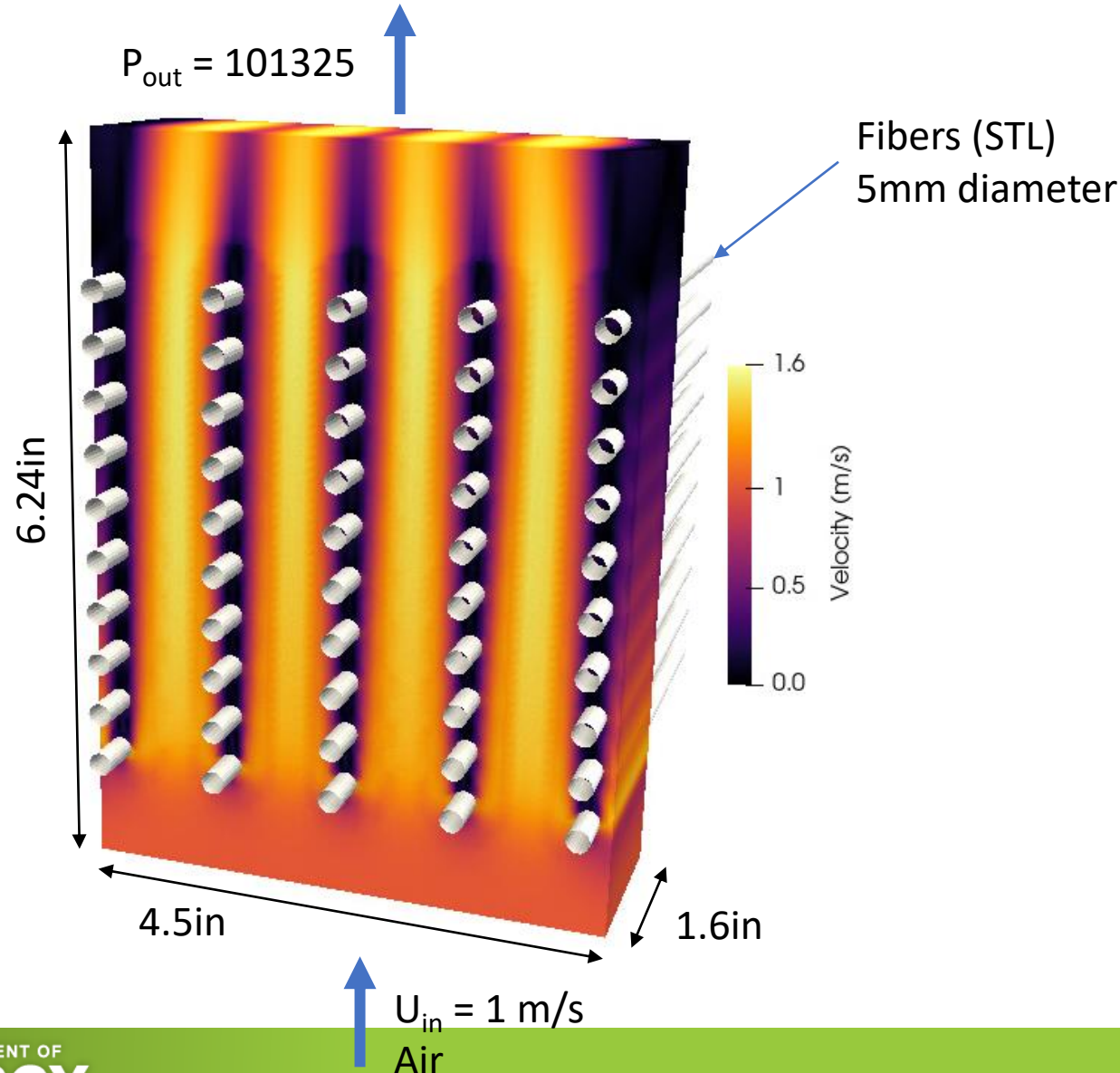
Film cooling

Score: 0.627



$3 \times 3 \times 3 \times 3 = 81$ dims

Base OpenFoam model



Solver: simpleFoam (steady state)

Mesh: 210k cells

Turbulence: kOmegaSST

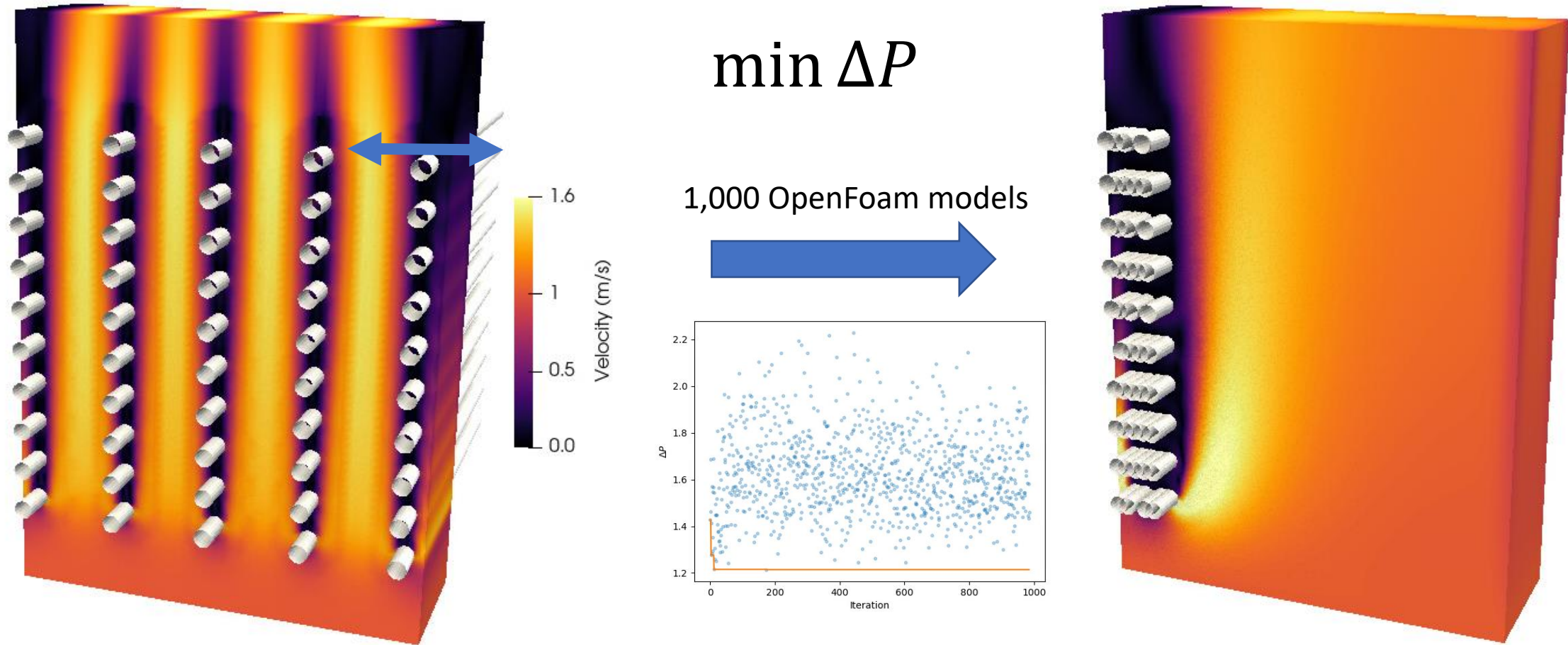
Runtime: 4 Cores, meshes in 20s,

runs in 3.5 minutes

10 x 5 = 50 dims

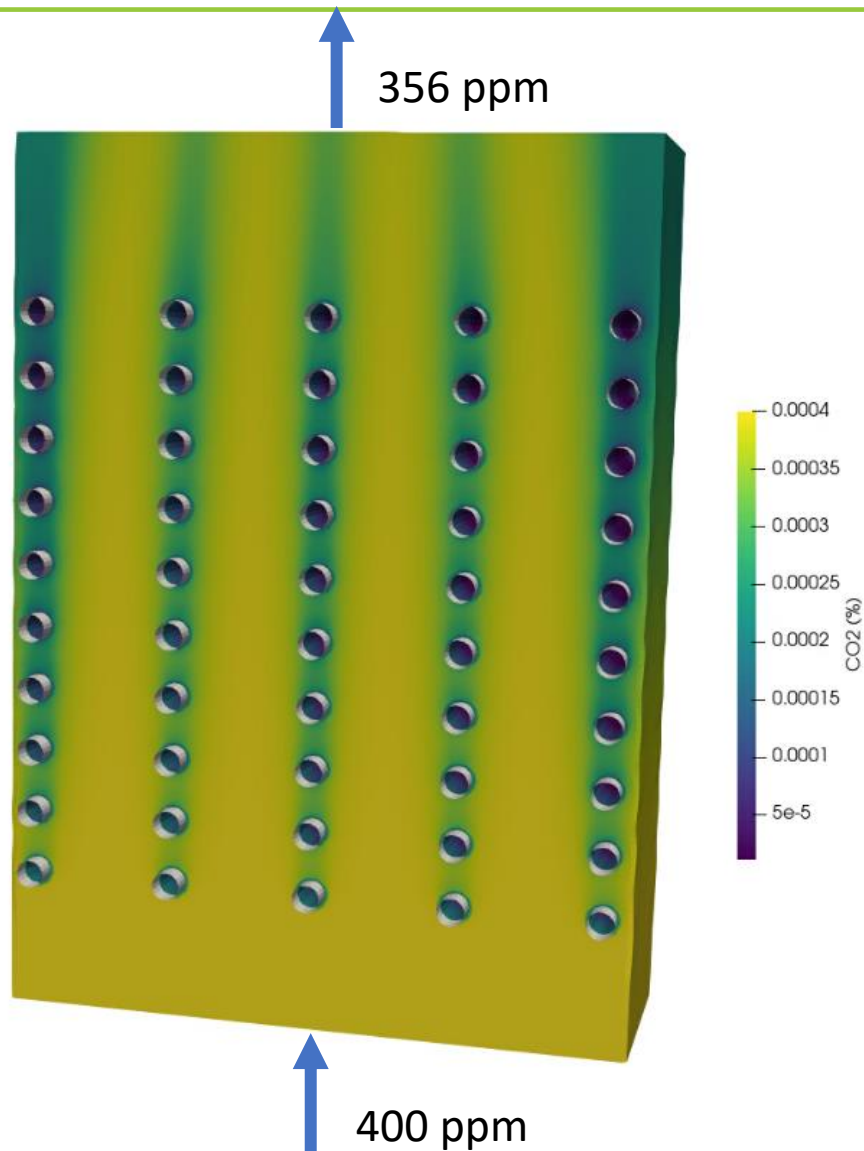
Optimization results: min ΔP

Fixed fiber count, allow the positions to move in the lateral (x) direction



It works! Minimizes pressure drop by condensing all the geometry to one side, not good for surface reactions!

Add Reactions!

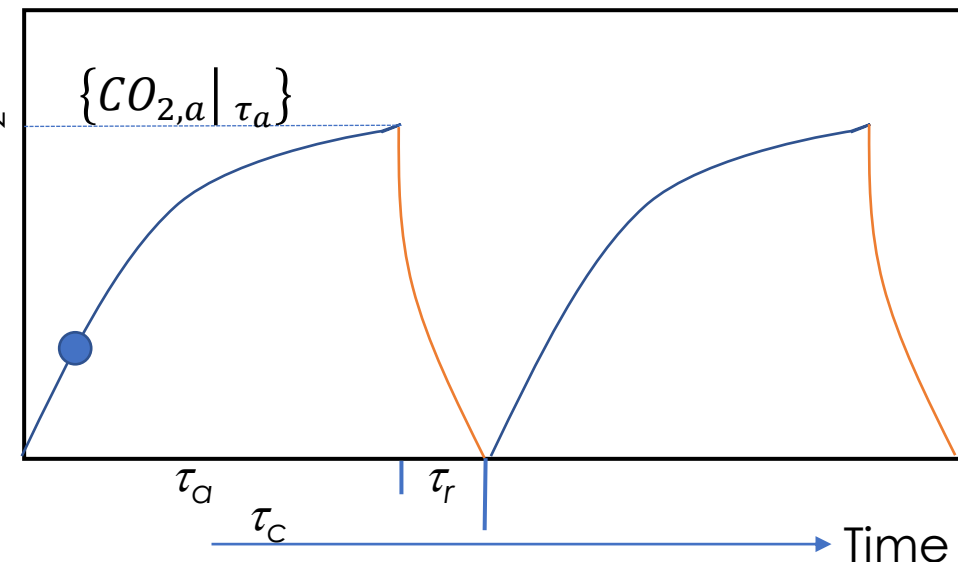


Fake reactions with a “CO₂” scalar
Use a “Mixed boundary condition” to mimic absorption

$$\phi_f = w\phi_{ref} + (1 - w) (\phi_c + \Delta\nabla\phi_{ref})$$

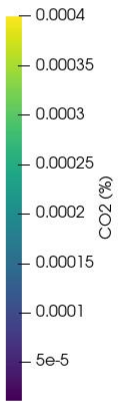
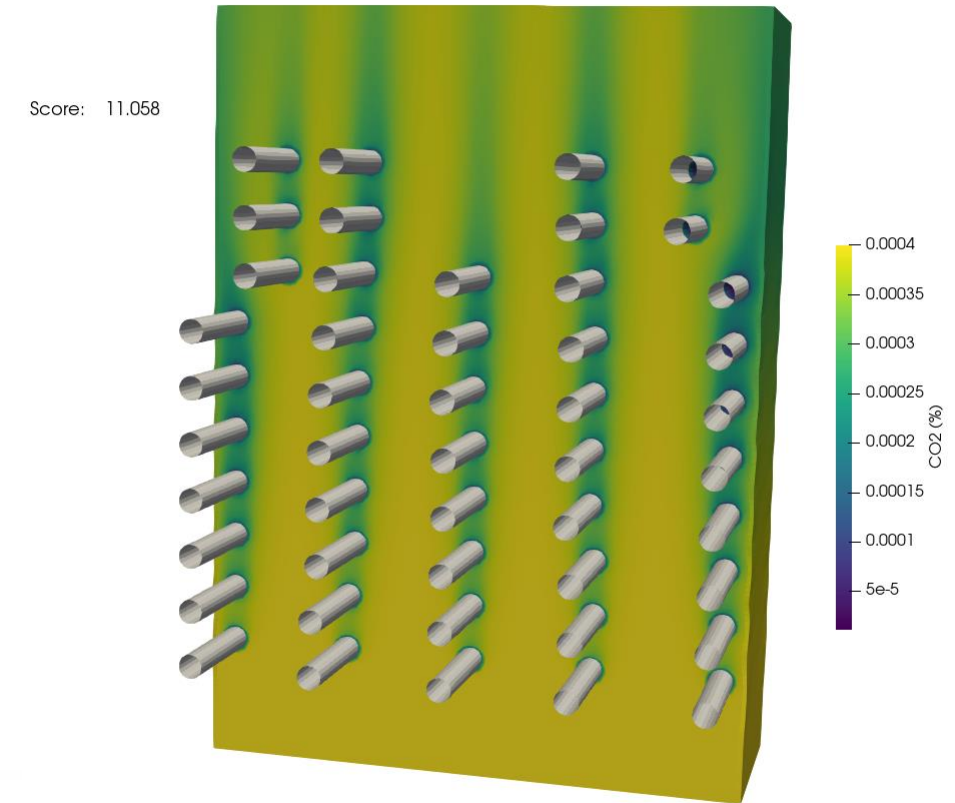
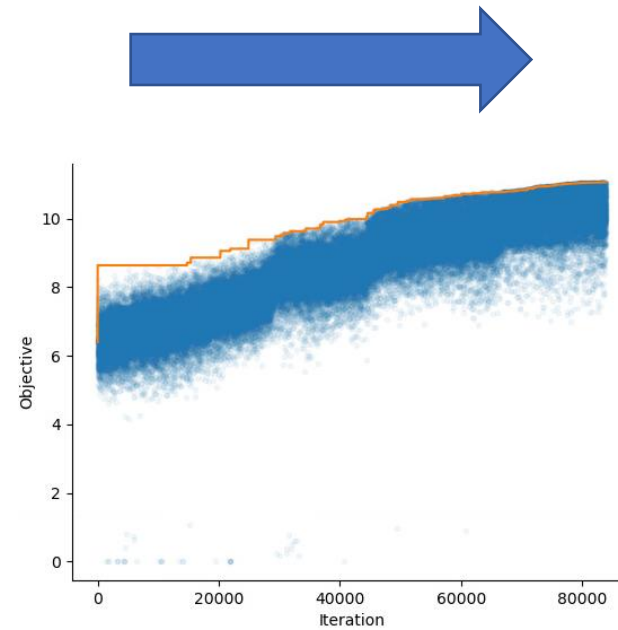
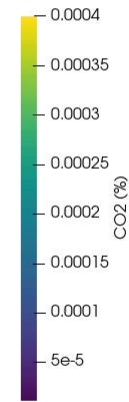
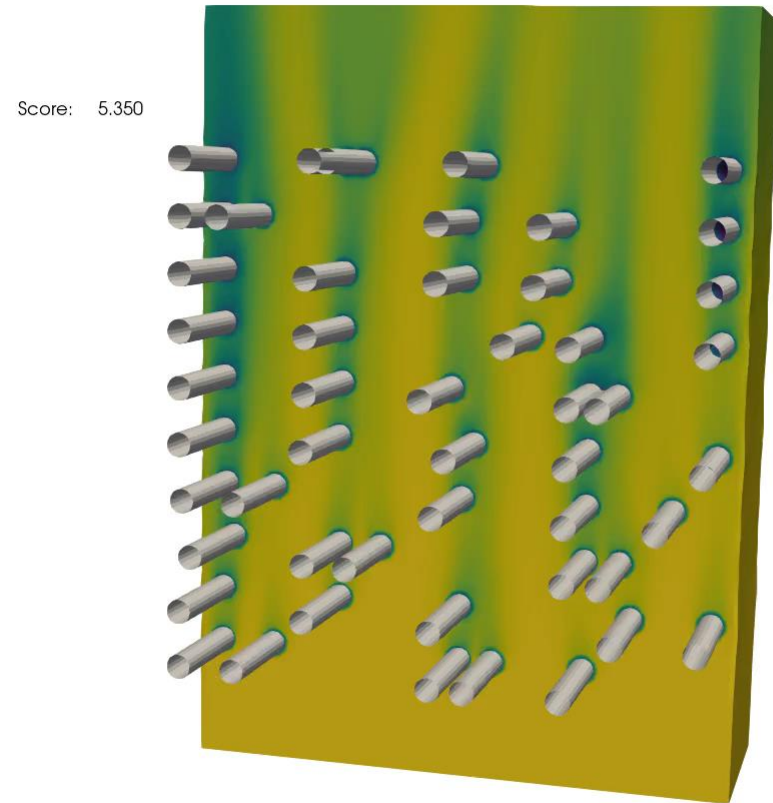
- ϕ_f = face value
- ϕ_c = cell value
- ϕ_{ref} = reference value
- Δ = face-to-cell distance
- w = value fraction

Cumulative CO₂ Adsorbed



Optimization results: with reactions

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

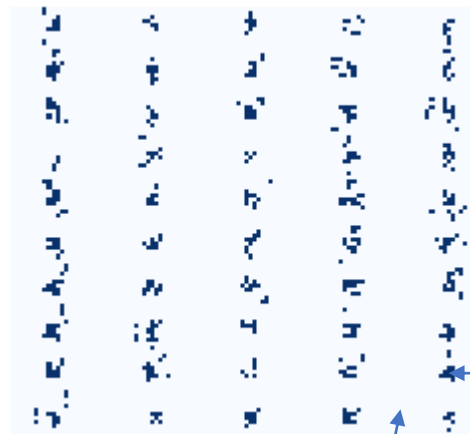


Binary Level set + GA

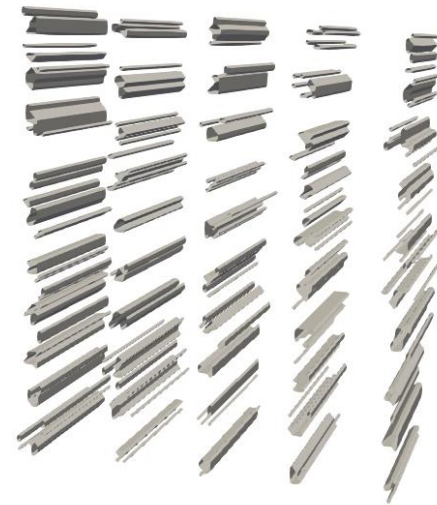
112 x 104 binary array

STL file

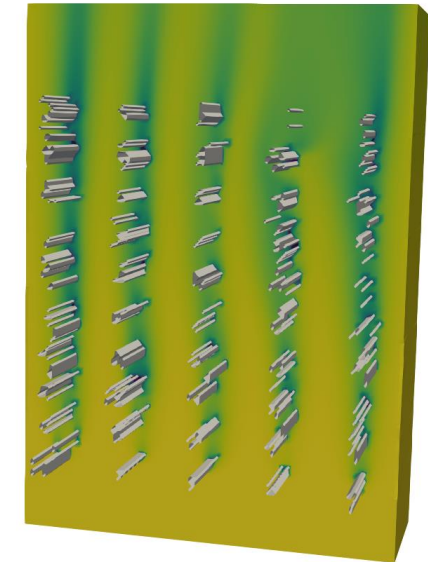
Model



contoured

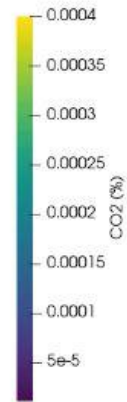
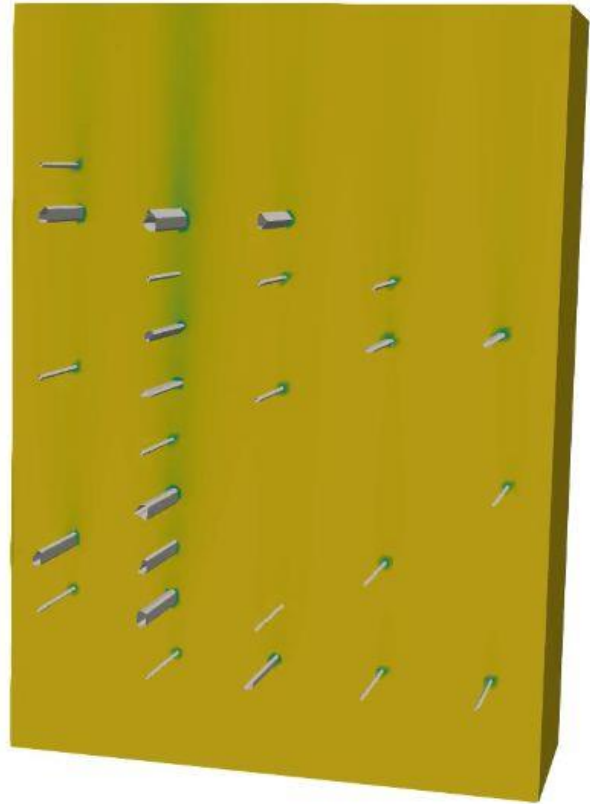


Mesh

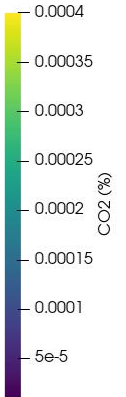
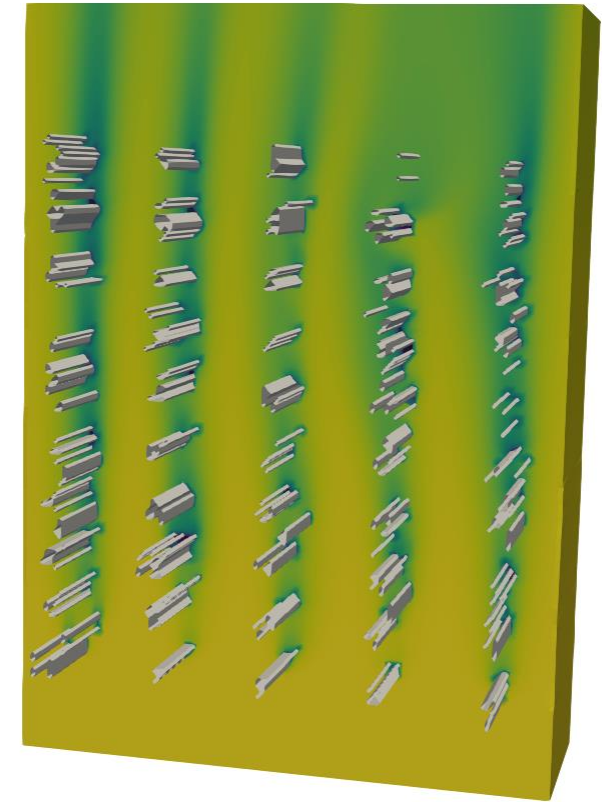
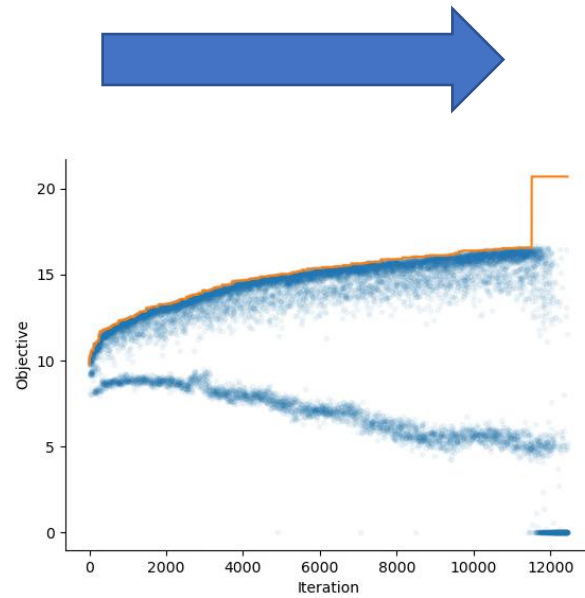


Binary Level set: Results

Score: 5.156

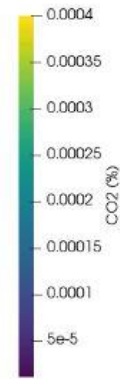


Score: 20.693

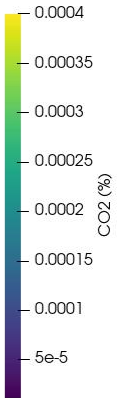
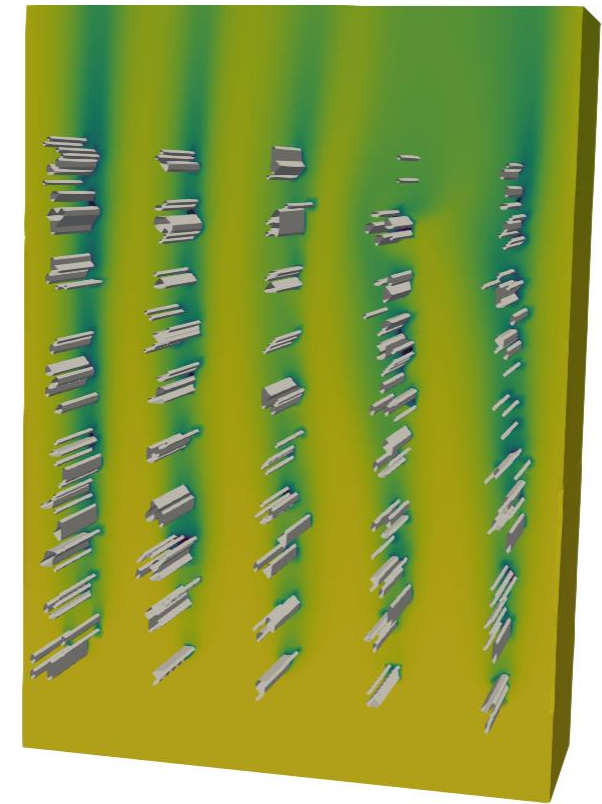
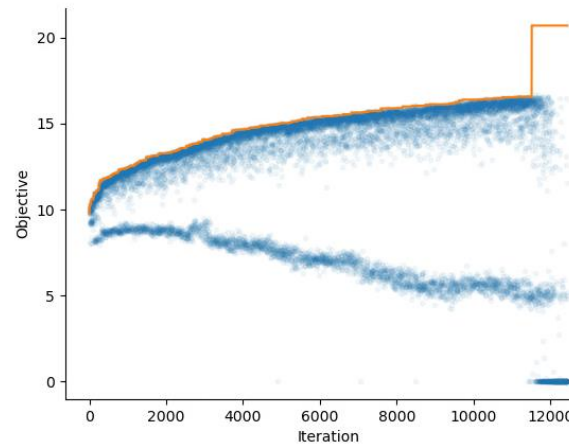


Binary Level set: Results

Score: 16.020

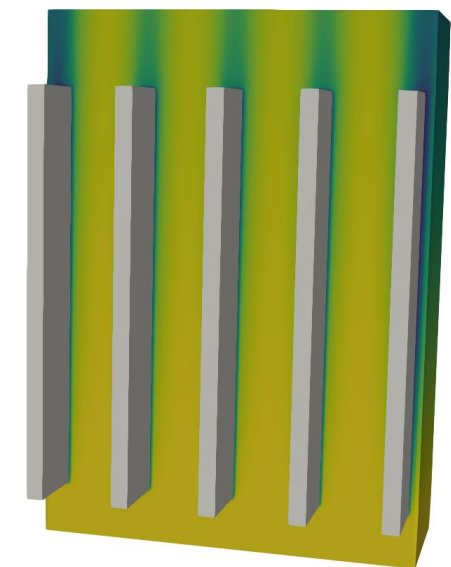


Score: 20.693



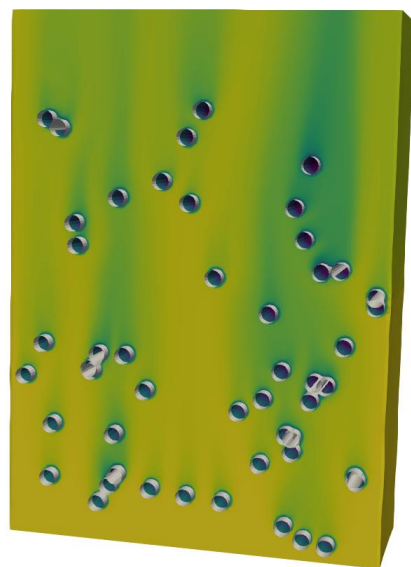
What's the best configuration?

Algorithmic



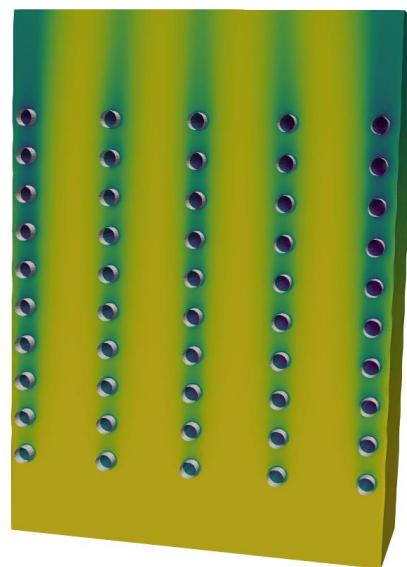
Score 18.1

Plates



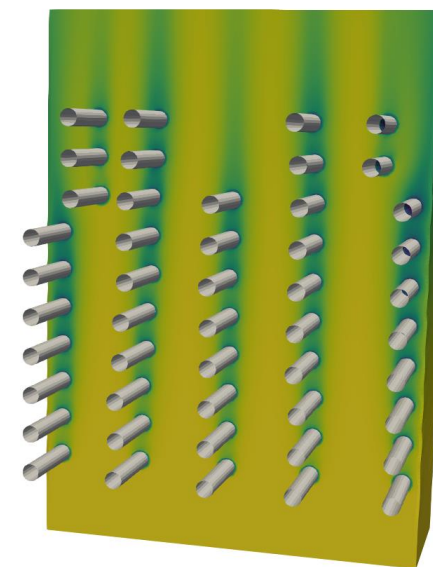
4.0

Random tubes



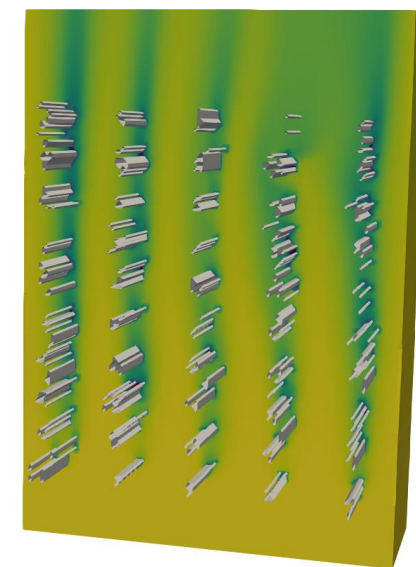
10.2

Structured tubes



11

Optimized tubes

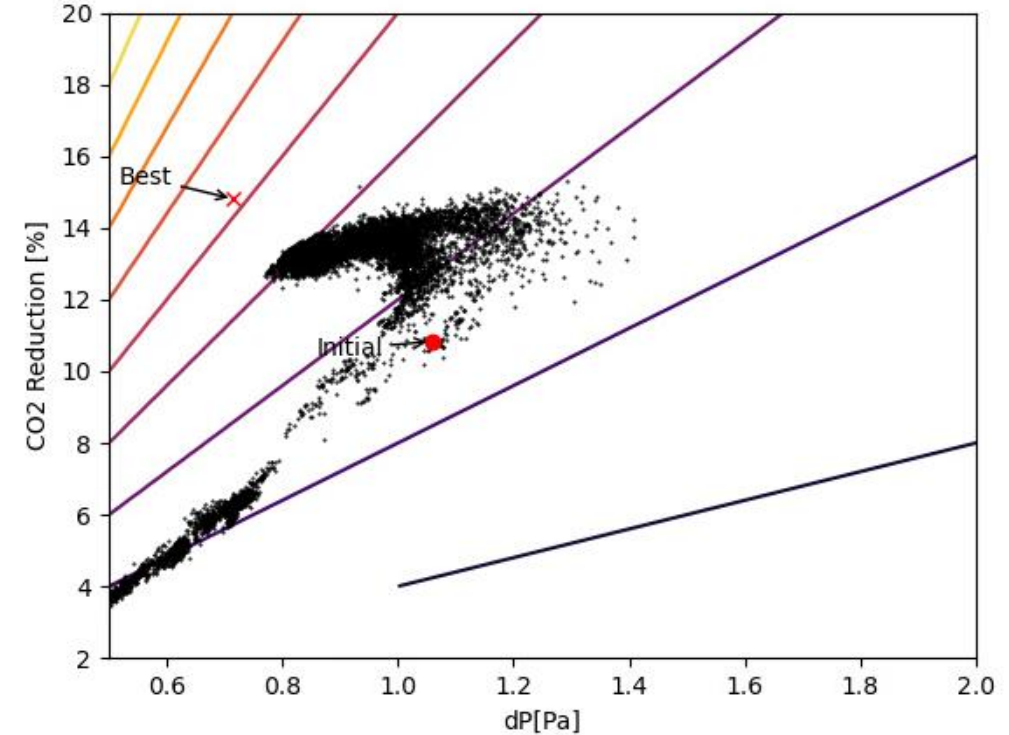


20.7

Free form

Summary

- Need to reduce energy consumption → reduce pressure drop
 - Use generative algorithms to optimize the design
 - Successfully ran OpenFoam simulations of the lab scale test unit geometry
- Next steps
 - Refine reactions in OpenFoam model to calculate more realistic objective function
 - Build and test promising design candidates
 - Validate optimization process with experimental data
 - Extend to multi-objective



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