Antifouling *active surface*-by-design from automated Bayesian optimization

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Presentation @ Antifouling Meeting[1]

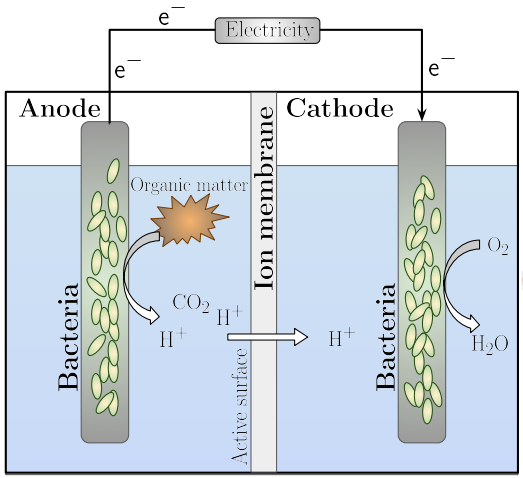
MAE, Cornell University

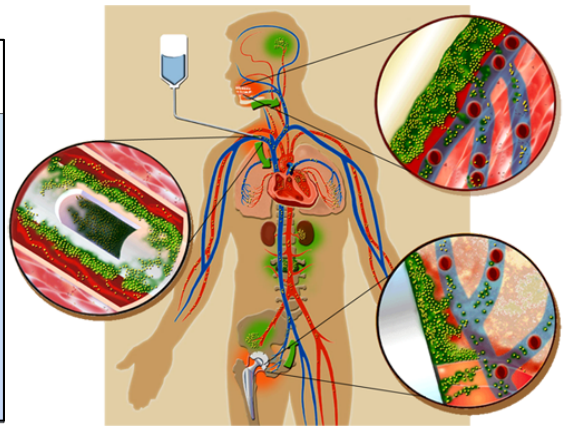
April 26, 2022

[1] work supervised by Prof. Jingjie Yeo

Backgrounds

Biofouling is a pain in ocean, energy engineering, biomedical treatments, etc. We hope to provide a **digital solution** for this hard problem.





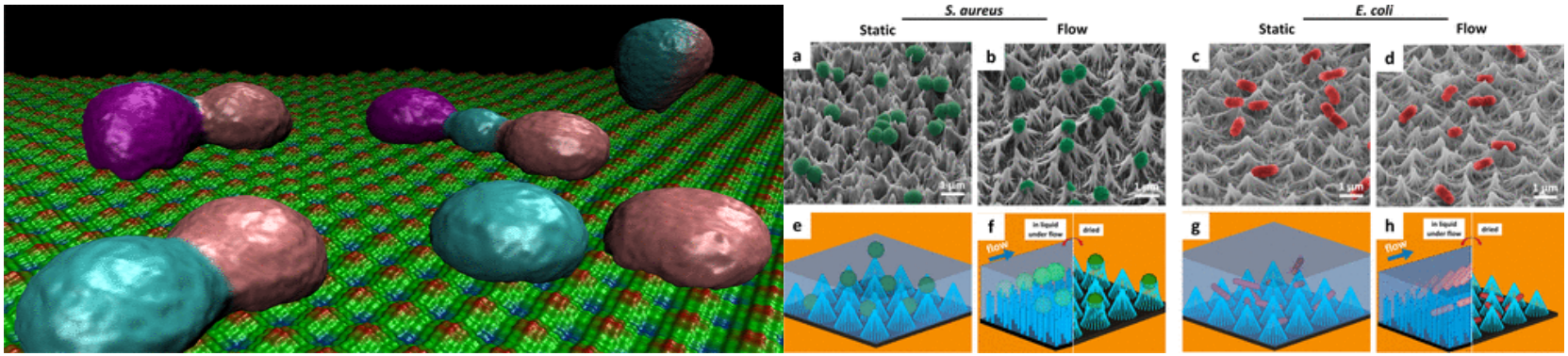
Objective

Use **optimization** and **multiphysics simulations** to design active surfaces with antimicrobial properties under **different loading environments**.

[1] https://www.clubmarine.com.au/exploreboating/articles/32-3-Keeping-A-Clean-Bottom [2] https://www.cs.montana.edu/webworks/projects/stevesbook/contents/chapters/chapter005/section002/blue/page005.html

Backgrounds

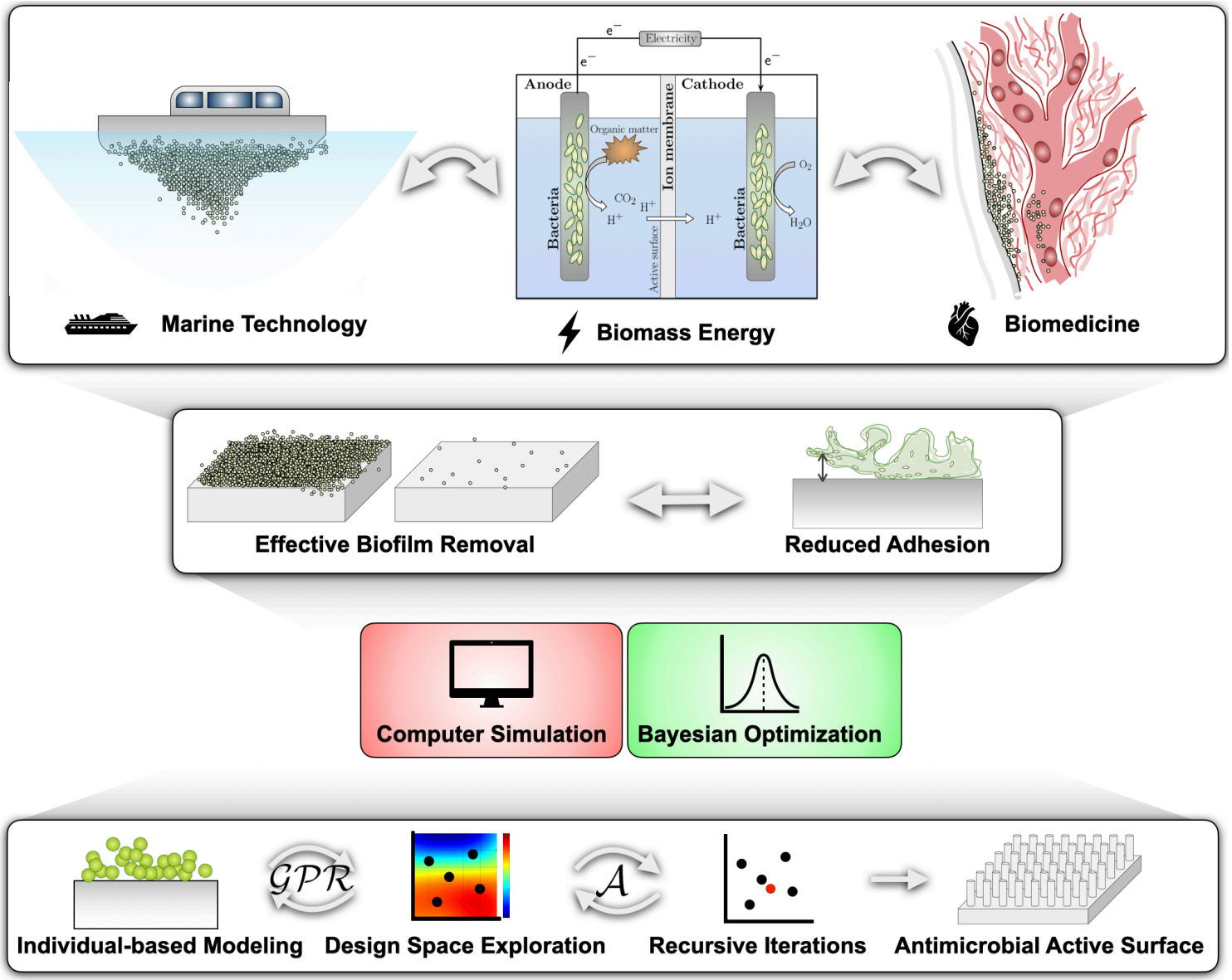
- Hydrophobic nanosurfaces (coatings) for antifouling has been experimentally verified in multiple works.
- Bayesian optimization has been shown successfully implemented in materials design and topology optimization.
- Individual based modeling[2] is currently one of the most successful method for accumulating M&M properties of biofilm modeling.



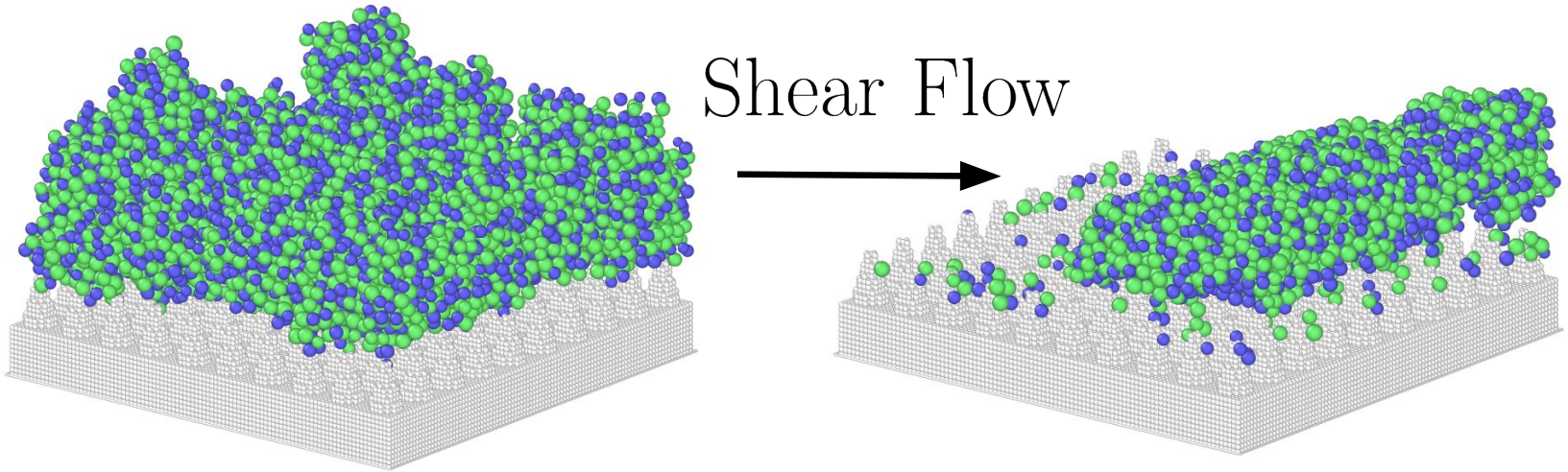
Zhang et al., *Langmuir*, 2019; Hizal et al., *ACS Appl. Mater. Interfaces*, 2017.

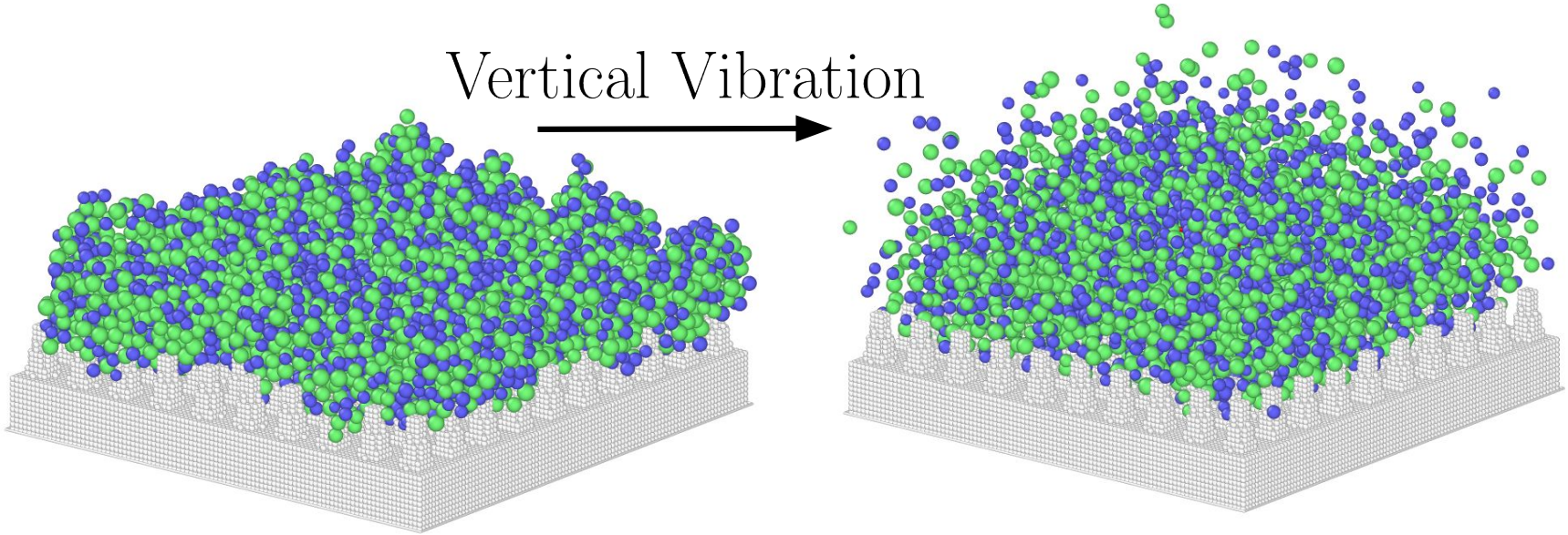
[2] https://hanfengzhai.net/file/Biofilm_review.pdf

Basic workflow

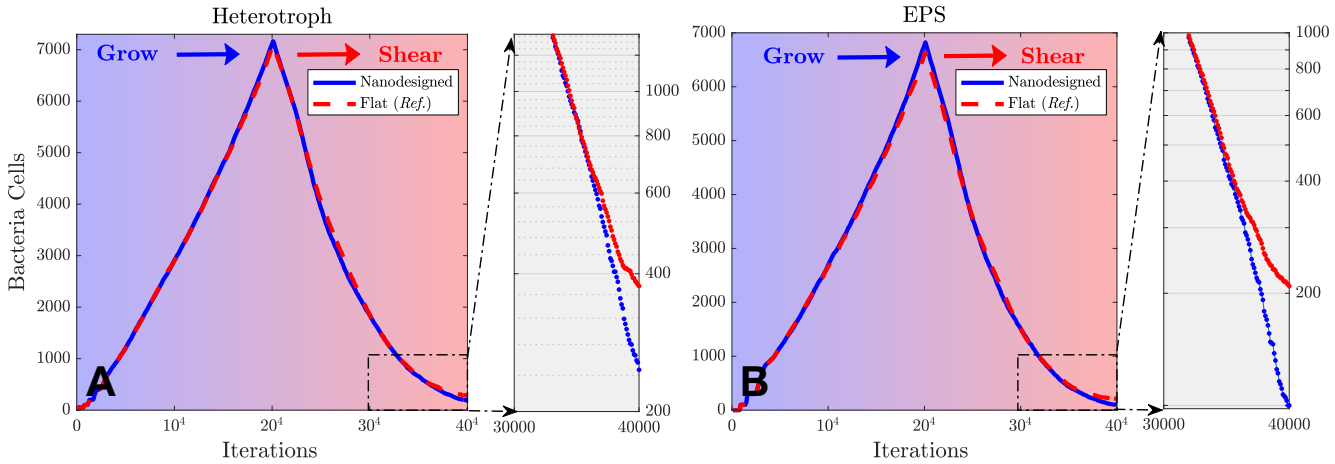


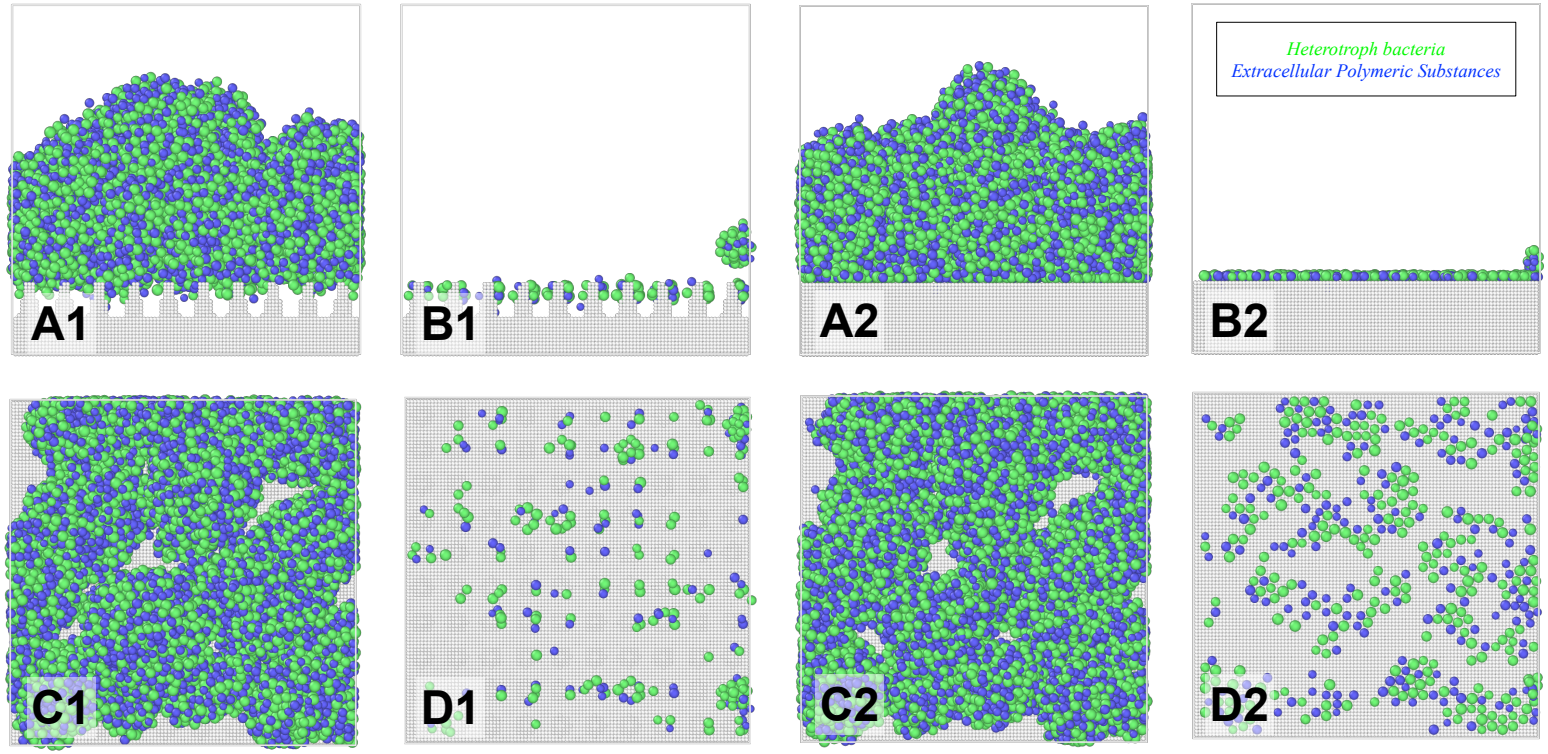
Biofilm removal: shear and vibration



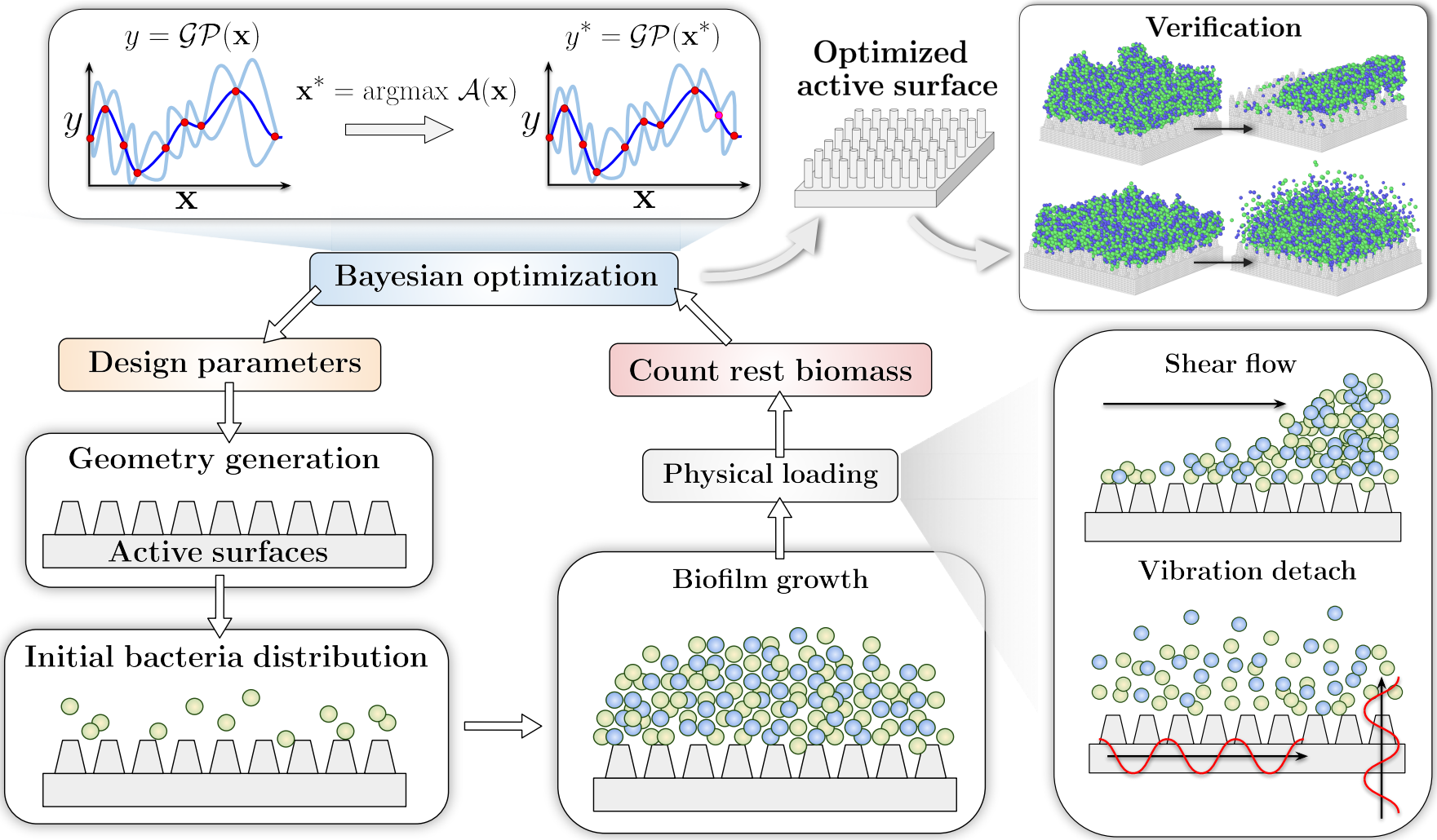


Why this kind of surface works at all?

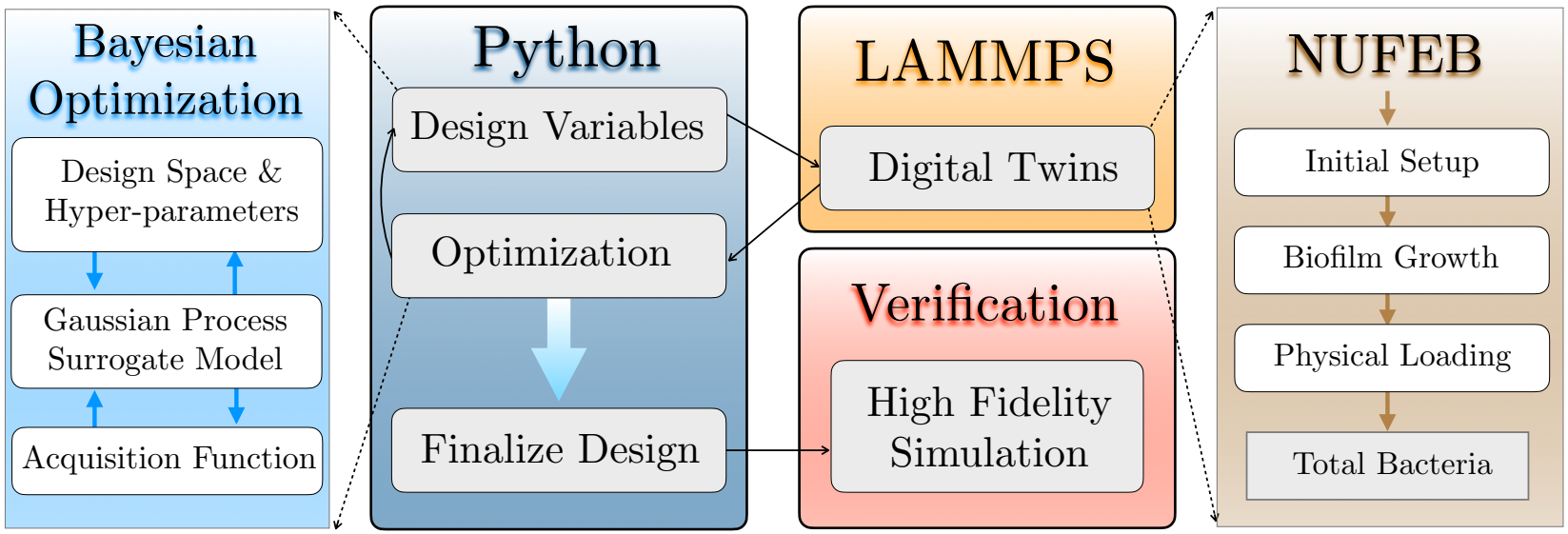




Bayesian coupled workflow for materials design



Optimization workflow

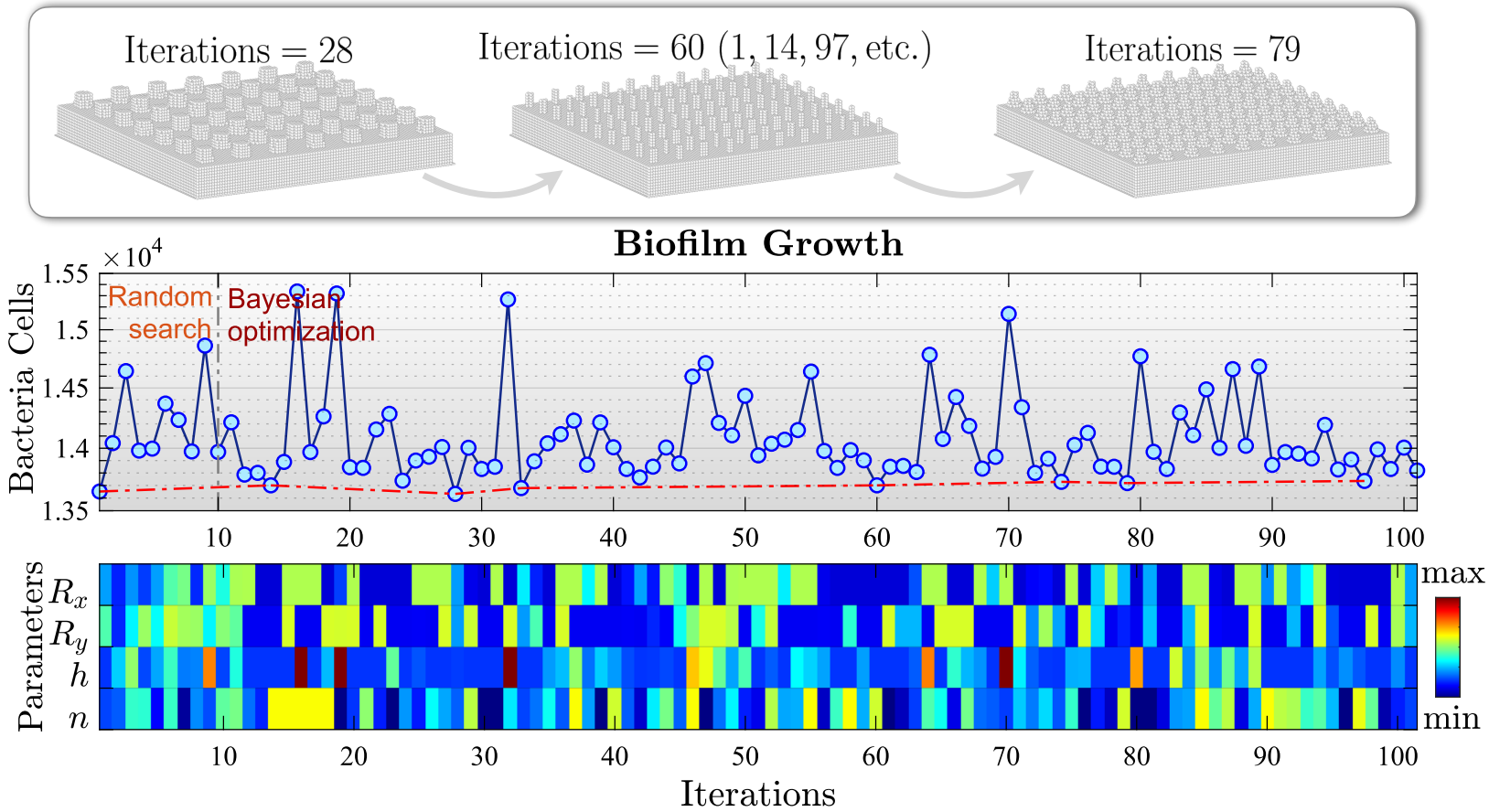


Technical Implementation

1. The whole optimization workflow is dependent on Python-LAMMPS interface.
2. Calculation on 100 CPU cores usually requires approximately 30 hours.
3. Variables are passed from randomization in Python to LAMMPS as a string (%s).

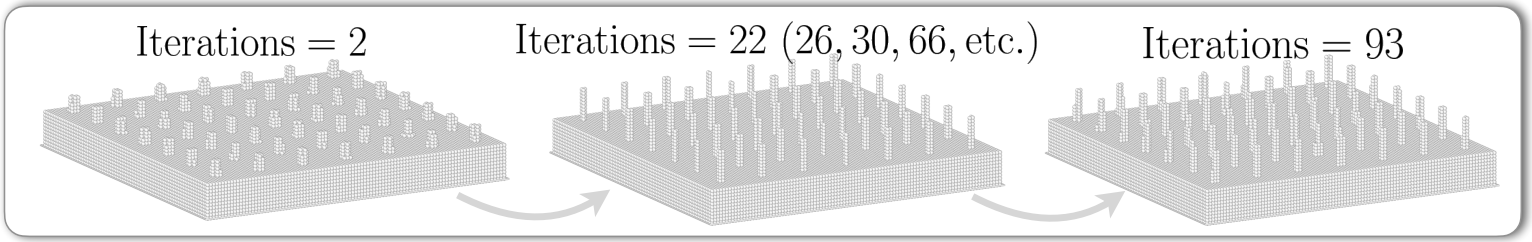
Results: pure biofilm growth

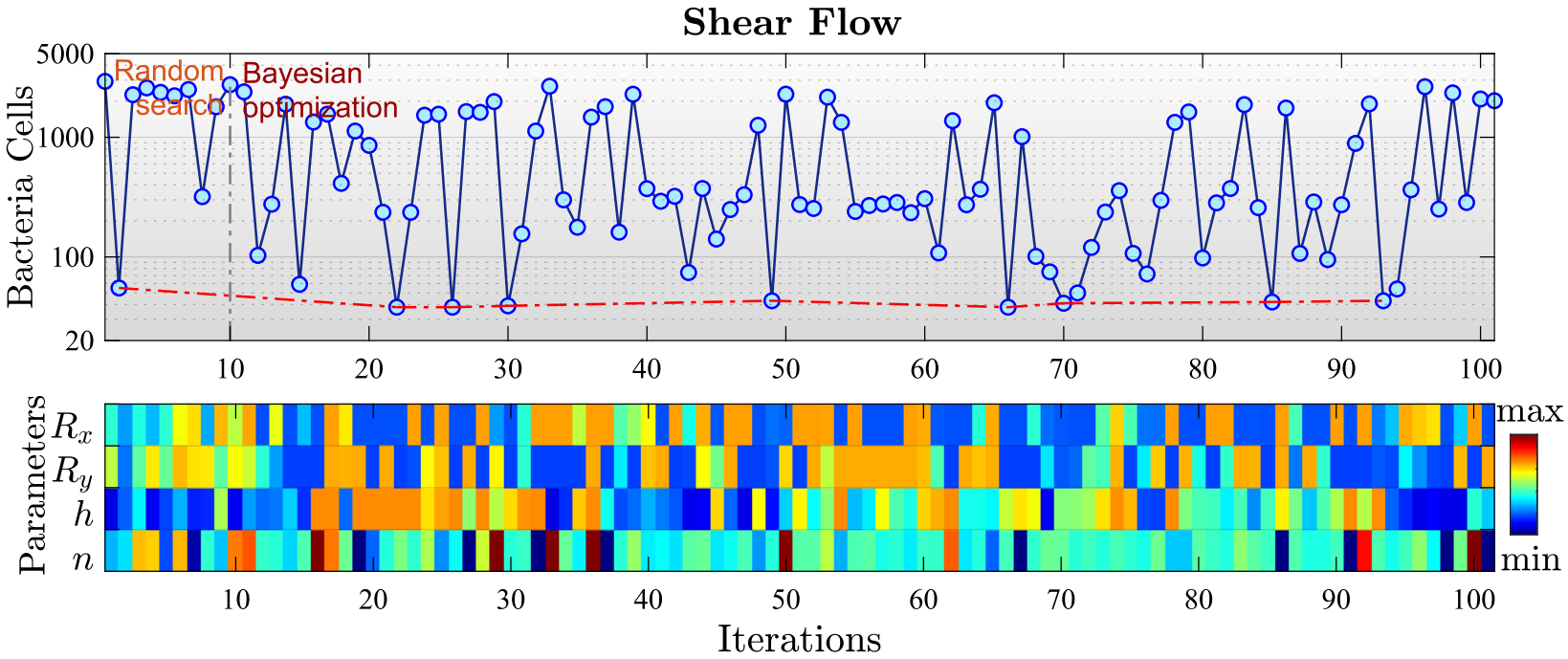
The active surfaces with shorter cones and mild thick shapes seem to effectively resist biofilm growth.



Results: shear flow detachment

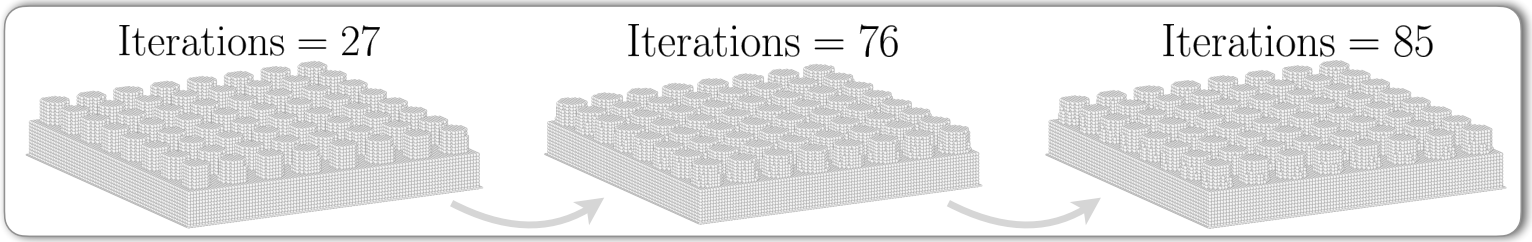
For the shear flow biofilm detach, a "thin pillar" –shaped cone designs shows extraordinary biofilm removal effect.

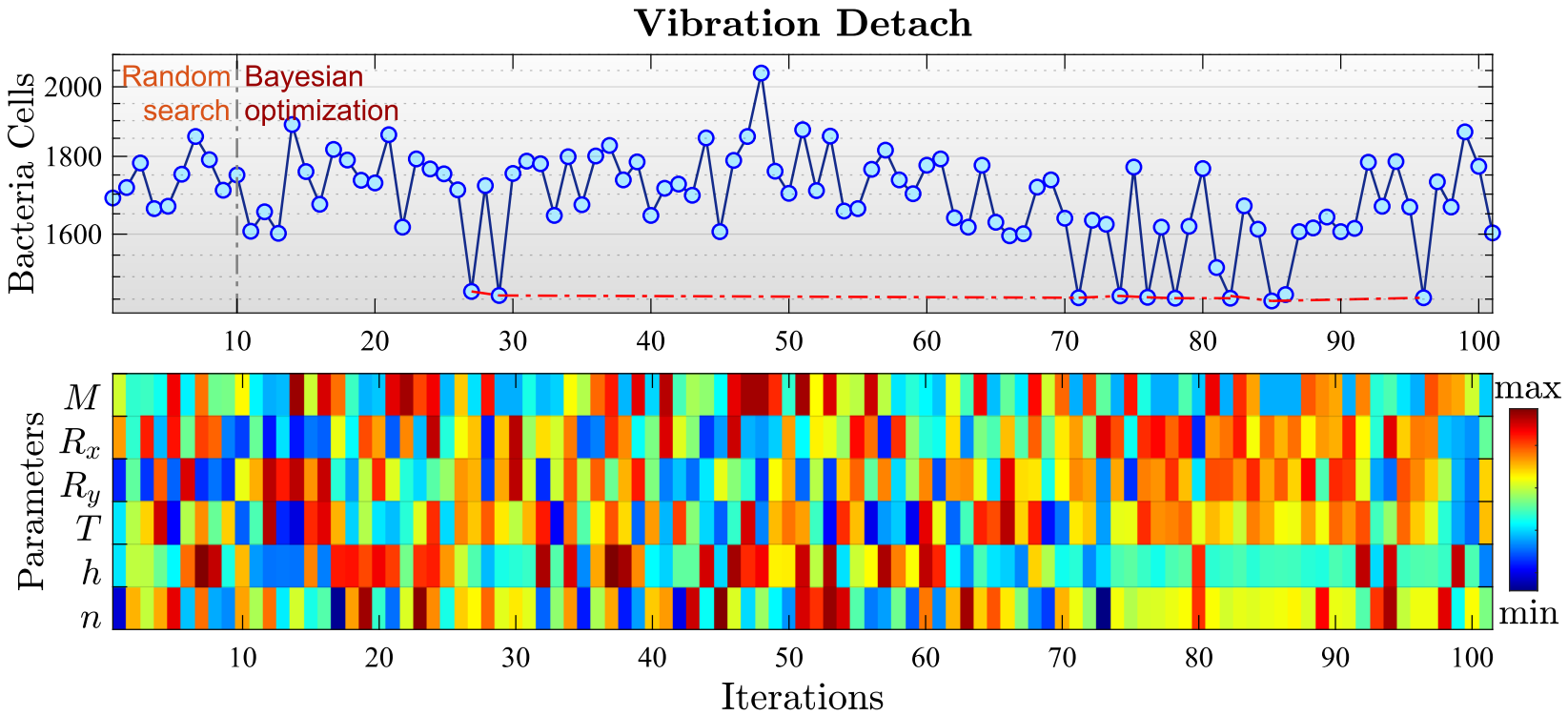




Results: vibration detachment

Strangely, but not strangely, for the vibration case, all the optimized active surfaces tend to exhibit very similar structures.





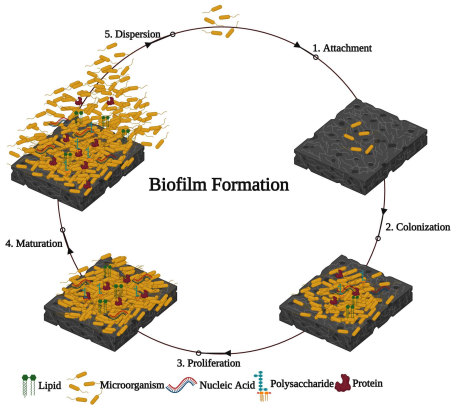
Summary & Conclusions

- The aim of this study is to present a **digital** solution for materials design targeting antifouling problems with **low cost** and **high efficiency**.
- An automated **optimization** workflow enabled by discrete element **multiphysics simulation** is presented for designing new antimicrobial materials.
- On resisting just the maturation and growth of biofilm, a topology with a shorter and mild thickness of the cones are generated from the optimization.
- For shearing, a **slim pillar-like topology** is generated from the optimization.
- For vibration, thick trapezoidal cones are found to be optimal.

Potential Problems & Future Directions

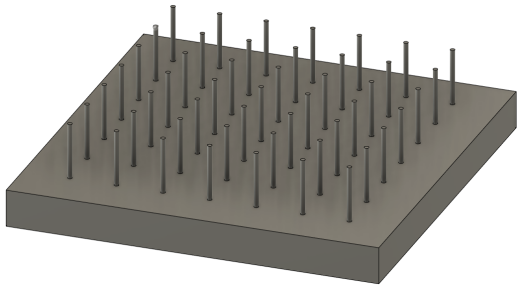
- Sensitivity of initial values & parameters.
- Comparison with flat surfaces for each optimal design.
- Parameters tuning in Bayesian optimization, i.e. κ (ucb), ξ (ei), etc.
- Inclusion of materials properties, i.e. constitutive models, thermal, electrical properties, etc.
- Experimental verification, polymer-based soft surfaces design, etc. (further collaborations)

- **Experimental Validation**



Srinivasan et al., *Front. Microbiol.*, 2021

- **3D Printing**



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Acknowledgement

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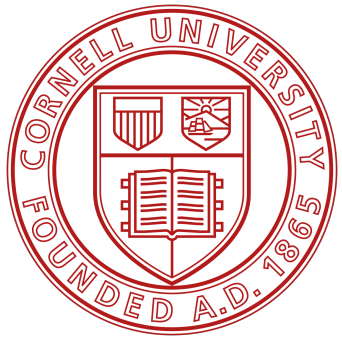

The End.

Any Questions...?