An automated Bayesian optimization workflow for antimicrobial nanosurfaces

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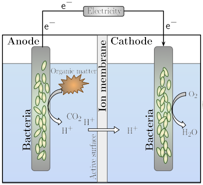
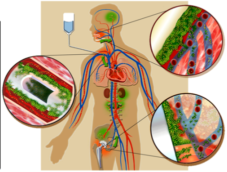
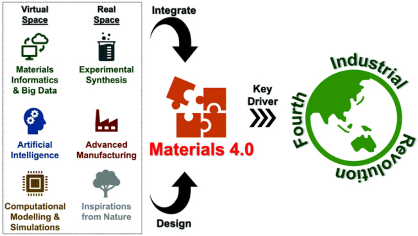
[1] work supervised by Prof. Jingjie Yeo

General Background

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







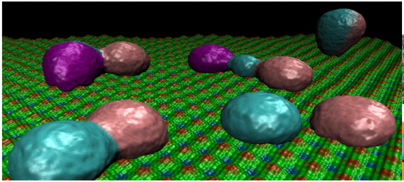
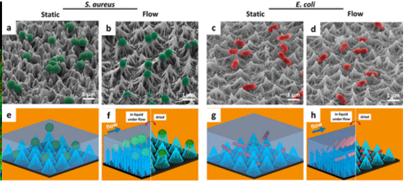
Digital twins + optimization

The recent "Materials 4.0 Initiative" drives huge innovations in materials-by-design with the "computational modeling + ML" paradigm in various fields.

[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

Inspirations & Technical Backgrounds

- The **super-hydrophobic surfaces** have been of interest for many years in the communities.
- Design the nanosurfaces (coatings) for antimicrobial properties have just recently been raised and the trend is growing drastically.
- **Bayesian optimization** for materials design is also becoming a new trend in the heated topic of ML algorithms for real-world problems.
- **Individual-based modeling**[2] is currently one of the most successful methods for accumulating M&M properties of biofilm modeling.

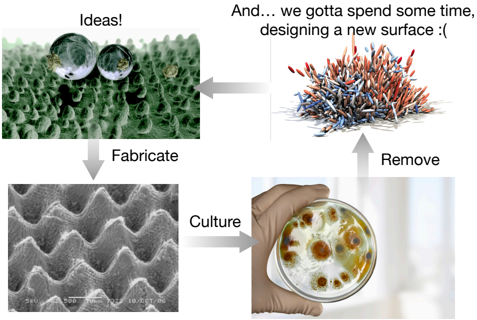



Zhang et al., *Langmuir*, 2019; Hizal et al., *ACS Appl. Mater. Interfaces*, 2017.

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

When there's a problem, there's a solution!

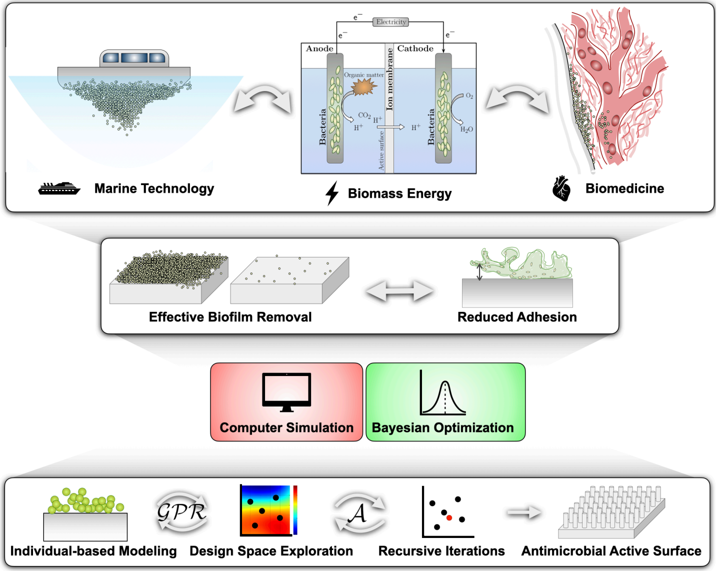
Traditionally, how do we solve this problem?



If you rich and got plenty of time, you fine... :)) But can we solve this problem in a more "efficient" way?

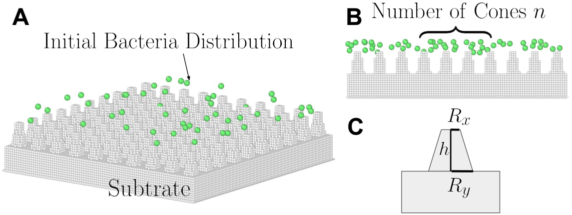
https://www.youtube.com/watch?v=HF4blivJQ6o
https://phys.org/news/2007-01-lotus-leaf-imitated-plastic-femtosecond.html
https://researchoutreach.org/articles/breaking-down-fort-combatting-clinical-biofilms/
https://www.ucl.ac.uk/~ucahppe/research.html

Basic workflow

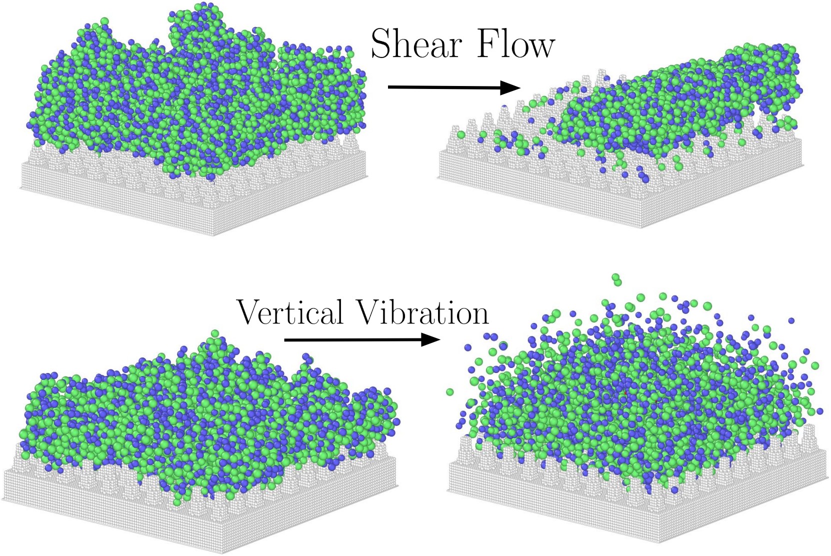


Numerical setup

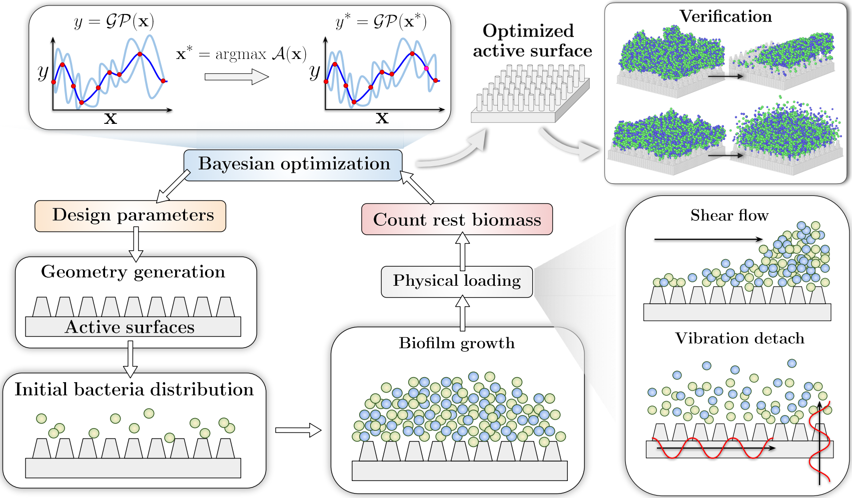
- **Geometric Design variables**: R_x, R_y, h, n
- **Simulation box**: Geometry: 4×10^{-3}m for x, y, z; *Boundary conditions*: fixed BCs on x, y, z; *Initial bacteria area*: 2×10^{-6}m
- **Bacteria cells**: *Initial No.*: 50; *Growth rate*: 0.00028; *Yield*: HET: 0.61 & EPS: 0.18. Monod growth model. HET: $K_s = 3.5 \times 10^{-5}$
- **Material properties**: *Heterotrophs*: $\rho = 150$; $d = 10^{-6}$; $m = 7.854 \times 10^{-17}$; *Substrate*: $\rho = 4410$; $d = 5^{-7}$; $m = 9.1875 \times 10^{-17}$.
- **Biofilm simulation**: *Grow*: $2 \times 10^4 (\times 10)$; *Shear*: $2 \times 10^4 (\times 2.5)$; *Vibration*: $1 \times 10^3 (\times 10^3)$;



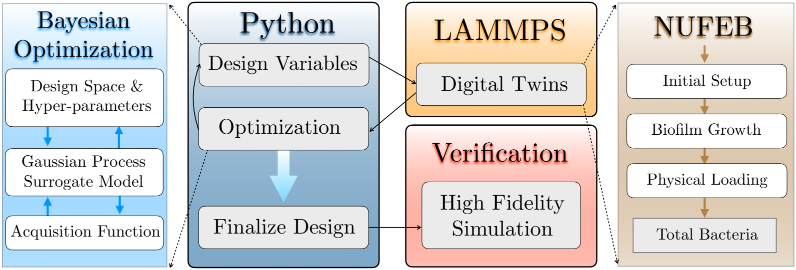
Biofilm removal: shear and vibration



Bayesian coupled workflow for materials design



Optimization workflow

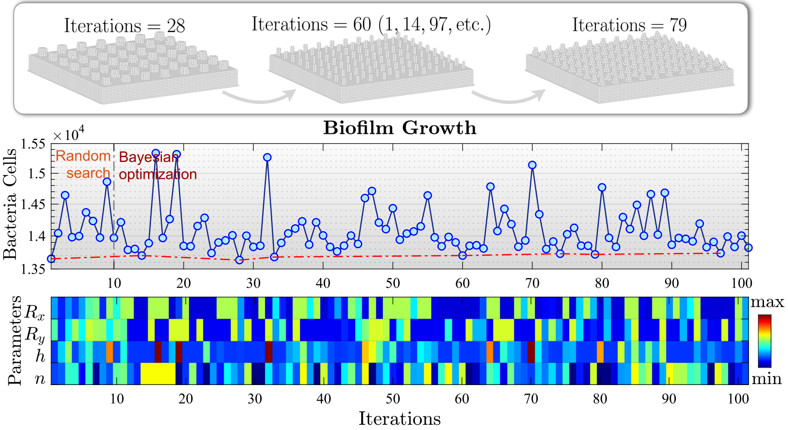


Technical Implementation

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).

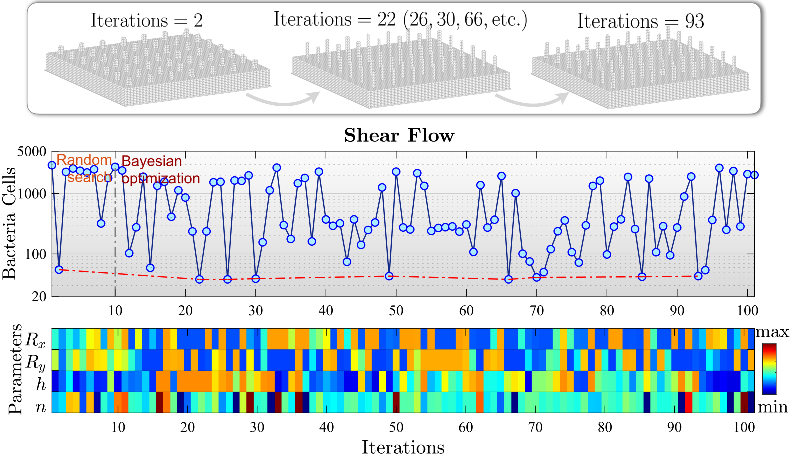
Results: pure biofilm growth

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



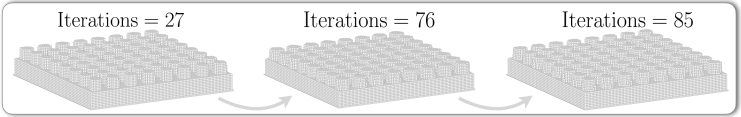
Results: shear flow detachment

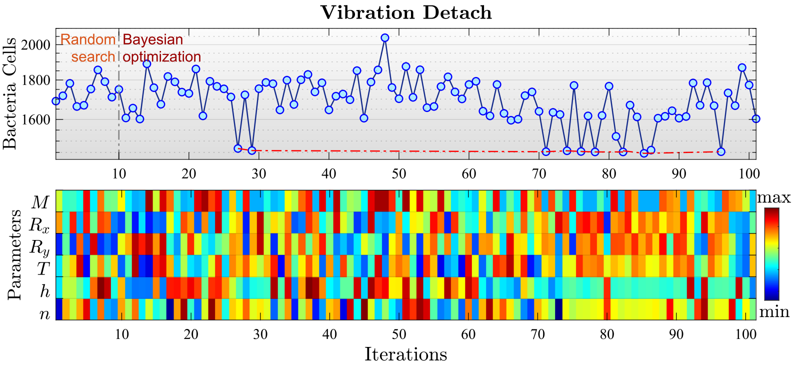
For the shear flow biofilm detach, a "thin pillar" −shaped cone designs shows extraordinary biofilm removal effect.



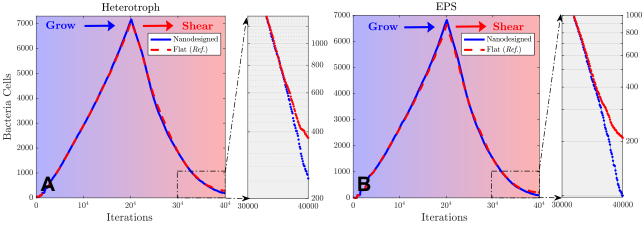
Results: vibration detachment

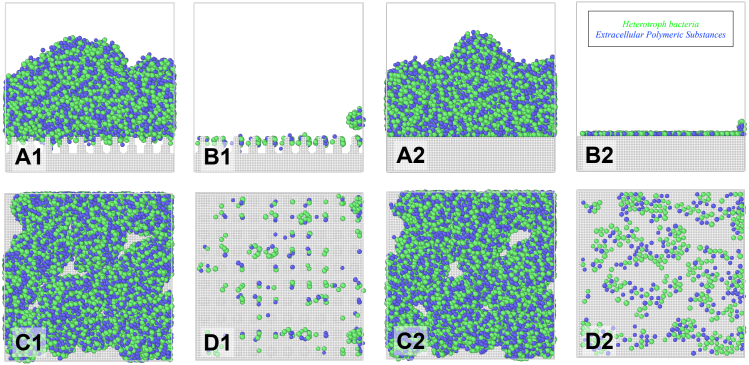
Strangely, but not strangely, for the vibration case, all the optimized active surfaces tend to exhibit very similar structures.





Verification

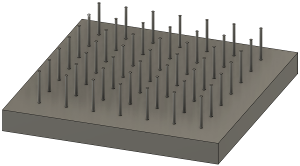




Summary & Discussions

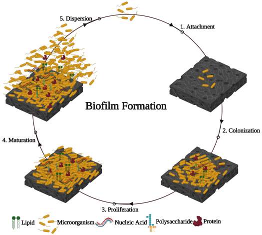
- This study presents a **digital solution** for materials design targeting antifouling problems with low cost and high efficiency.
- An automated **optimization workflow** enabled by discrete element multiphysics simulation is presented for materials design.
- Different **optimized geometries** based on different loading cases are generated from the workflow.

- **3D Printing**



Generated CAD file → 3D printing with hard materials for experimental verification

- **Experimental Validation**



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

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Acknowledgement

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Thanks for listening!

Any Questions...?