Bayesian Optimization Designs Metamaterials for Biofilm Control

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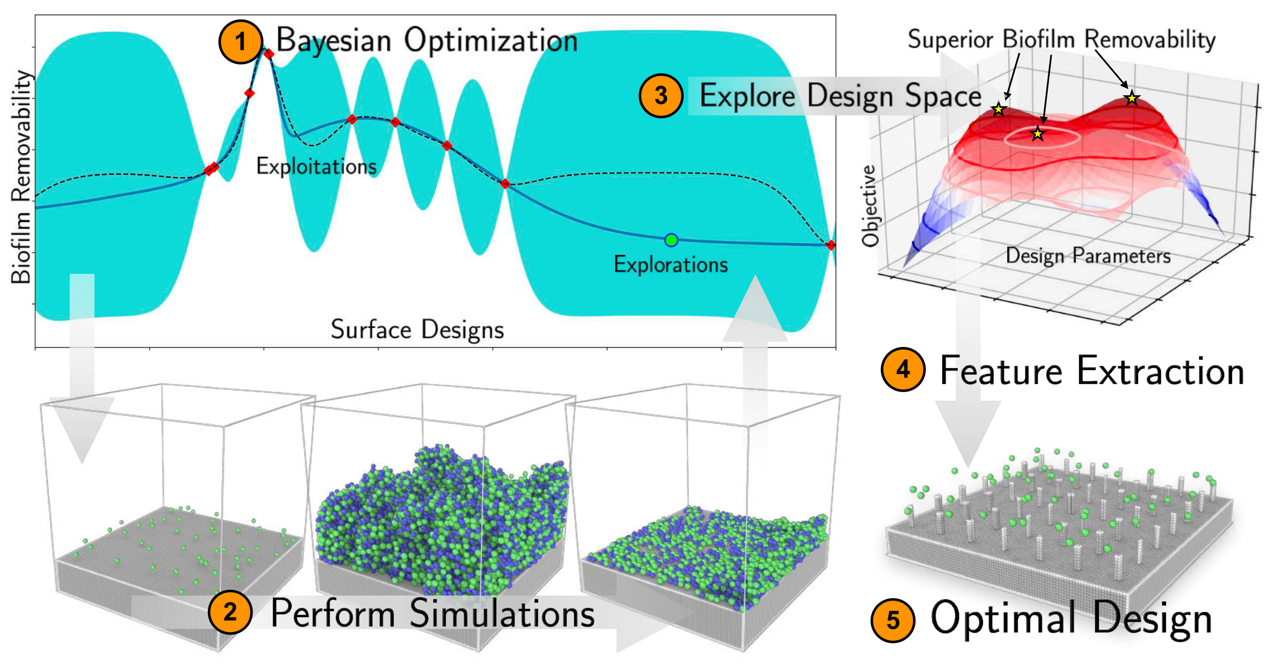
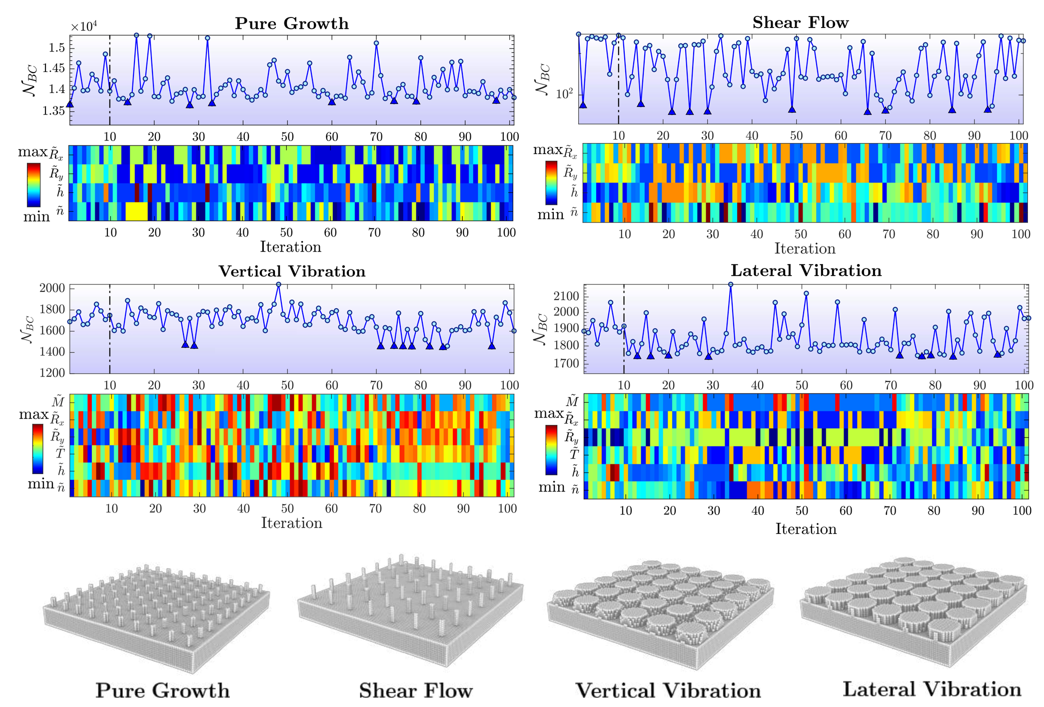
Research Overview & Objective

- We hope to design architectured materials in two and three dimensions for biofilm control, i.e., resist formation, accelerate transport, and storage, to utilize them as engineering living materials.
- We use individual-based modeling to simulate the growth and physics of biofilms and leverage Bayesian optimization to couple with our computational models for optimal design identification.

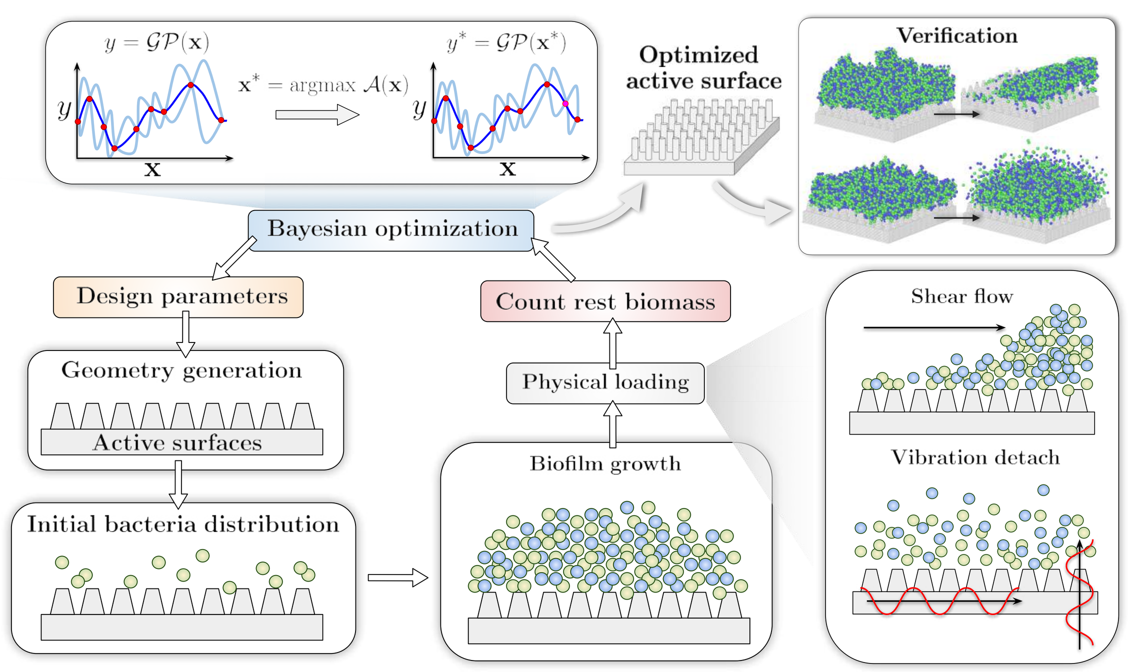
Bayesian Optimization for Antimicrobial Surface Design



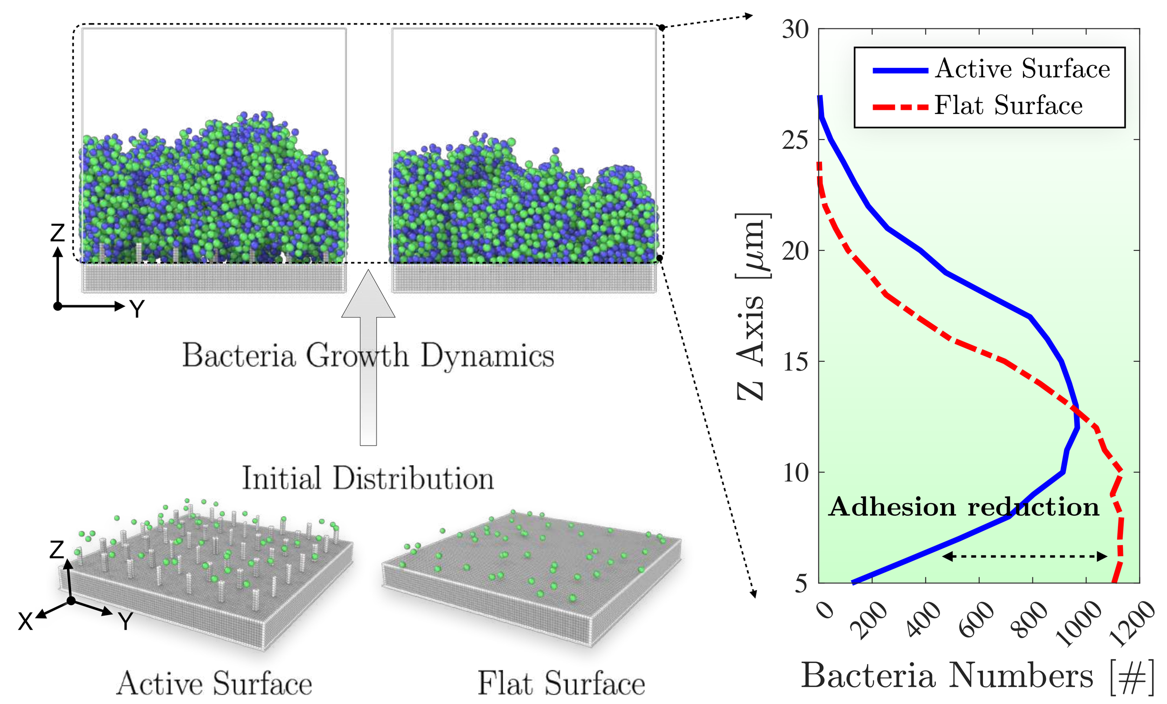
We hope to design nano/micro surfaces to resist biofilm attachment using computer simulations and machine learning techniques.



Our framework has successfully extracted optimal surface designs from automated simulations



We developed Bayesian optimization algorithms to generate optimal designs from simulations.



Based on our optimization results, we provide explanations of the biofilm removal mechanisms by looking at the adhesion mechanics.

← Scan the QR code to read the paper.
This work is published on *ACS Biomaterials Science & Engineering*.

Computational Modeling Plays a Central Role

Individual-based Modeling

The growth dynamics of biofilm are described by the equation:

$$\frac{dm_i}{dt} = \xi_i m_i \tag{1}$$

The particles are mechanically relaxed using the individual-based approach, solved via Newton's equation

$$m_i \frac{d\mathbf{v}_i}{dt} = \mathbf{F}_{c,i} + \mathbf{F}_{a,i} + \mathbf{F}_{d,i} \tag{2}$$

where m_i is the mass of a particle, and $\mathbf{v}_i$ is the velocity. Mechanical equilibrium is achieved when the average pressure of the microbial community reaches a plateau. The average pressure writes:

$$P = \frac{1}{3V}\left(\sum_{i=1}^{N} m_i \mathbf{v}_i \cdot \mathbf{v}_i + \sum_{i=1}^{N}\sum_{j>i}^{N} \mathbf{r}_{i,j} \cdot \mathbf{F}_{i,j}\right) \tag{3}$$

where V is the sum of the volumes of particles.

Bayesian Optimization

Considering an optimization objective $\hat{DS}(\mathbf{x}, \mathbf{p})$, where $\hat{DS}$ is evaluated at $\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_k \in \mathbb{R}^d$, we can obtain $[DS(\mathbf{x}_1), ..., DS(\mathbf{x}_k)]$ to construct a surrogate model for the design parameters with the correlated objectives.

$$\hat{DS}(\mathbf{x}_{1:k}) \sim \mathcal{N}\left(\mu_0(\mathbf{x}_{1:k}), \Sigma_0(\mathbf{x}_{1:k}, \mathbf{x}_{1:k})\right) \tag{4}$$

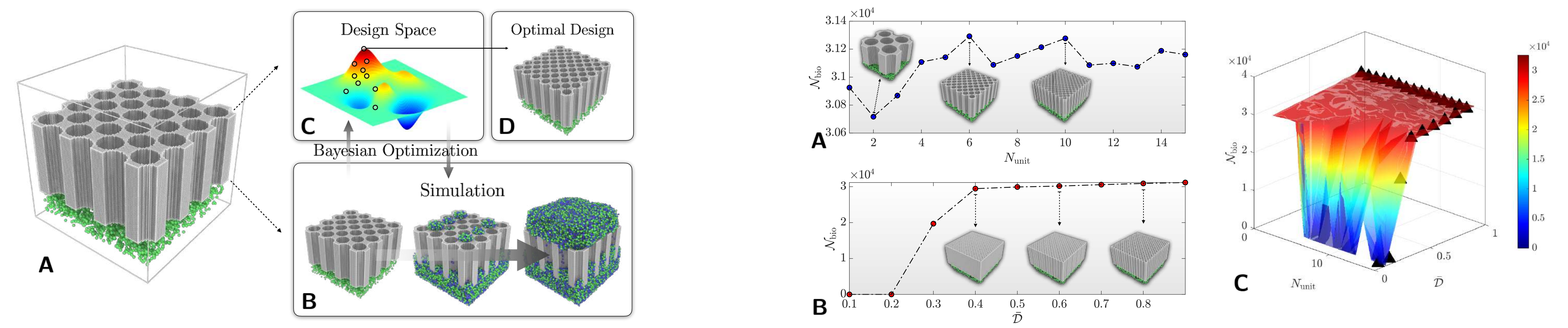
Taking our previous notation, the new observation is probed through the acquisition

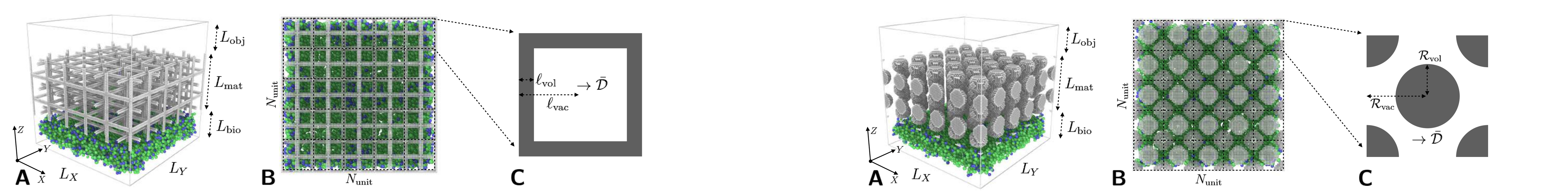
$$\mathbf{x}_k = \mathbf{x}_{l+1} = \text{argmax}_{x \in \frac{x}{\mathcal{X}_l}} \mathcal{A}\left(\mathbf{x}; (\mathbf{x}_l, y_l), \theta_m\right) \tag{5}$$

where the input space contains the evaluation of design variables: $\mathcal{X}_l := (\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_l)$. Take the GP Upper Confidence Bound (GP-UCB) as an example, exploiting the lower confidence bounds to construct the acquisition:

$$\mathcal{A}\left(\mathbf{x}; (\mathbf{x}_l, y_l), \theta_m\right) := \mu_l\left(\mathbf{x}; (\mathbf{x}_l, y_l), \theta_m\right) + \kappa\sigma\left(\mathbf{x}; (\mathbf{x}_l, y_l), \theta_m\right) \tag{6}$$

Bayesian Optimization for 3D Metamaterials





Design 3D porous metamaterials and conduct rigorous analysis on the design space's exploration.

Ongoing works and Future Directions

- Extend the formulated design optimization scheme to 3D metamaterials for enhanced biofilm transport and storage.
- Conduct rigorous and comprehensive analyses of the design optimization and characterize the physical coefficients and hyperparameters.
- Applying advanced machine learning techniques (normalizing flows, graph neural nets) for surrogate modeling of biofilm dynamics.

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