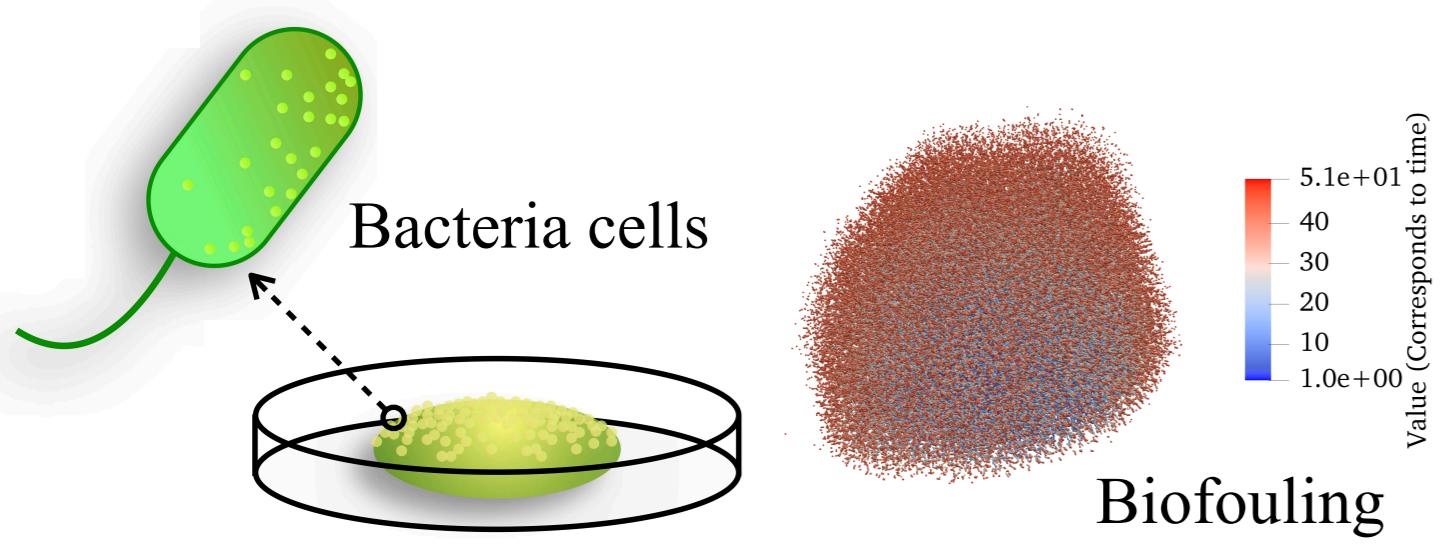


AI for Good + AI for Science

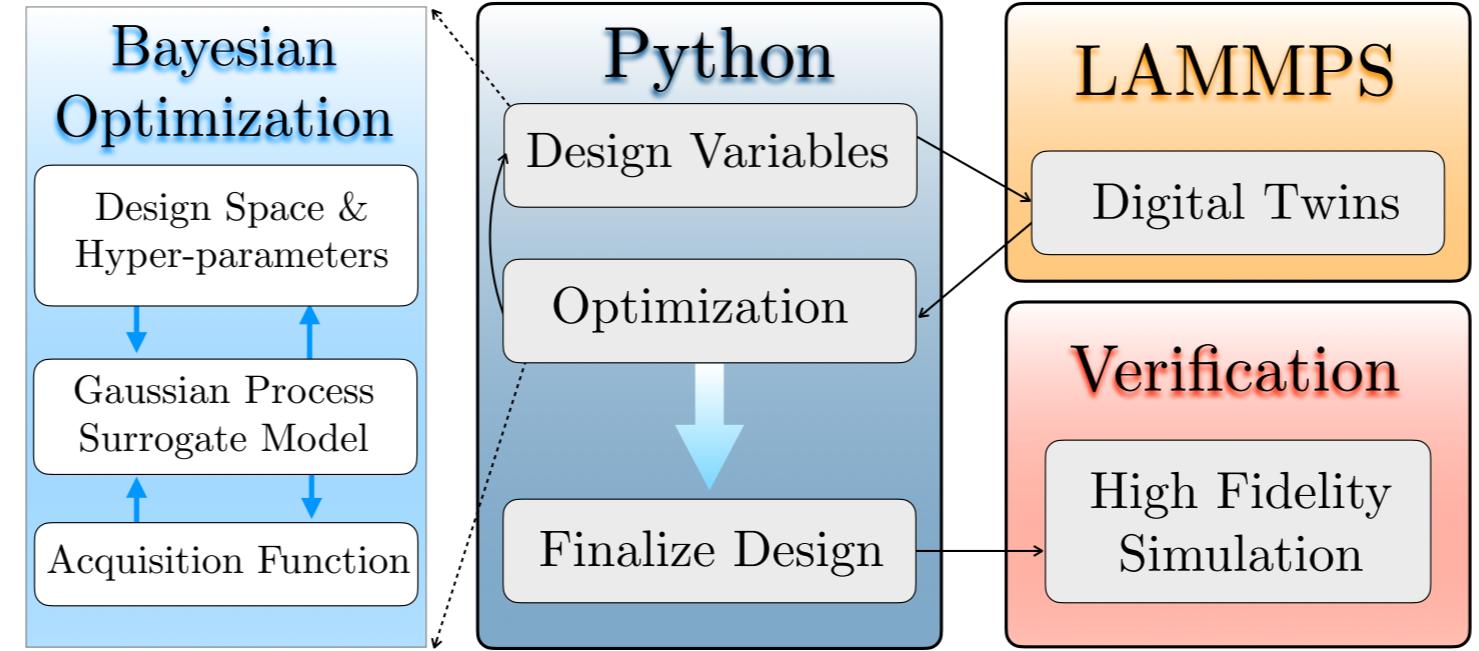
Designing next generation biocompatible materials with Machine Learning+Multiscale & Multiphysics Modeling

Goal & Objective



Biofilm stinks. We hope to find a way to get rid of it. Designing a new kind of nanosurface with computer simulation + ML is one.

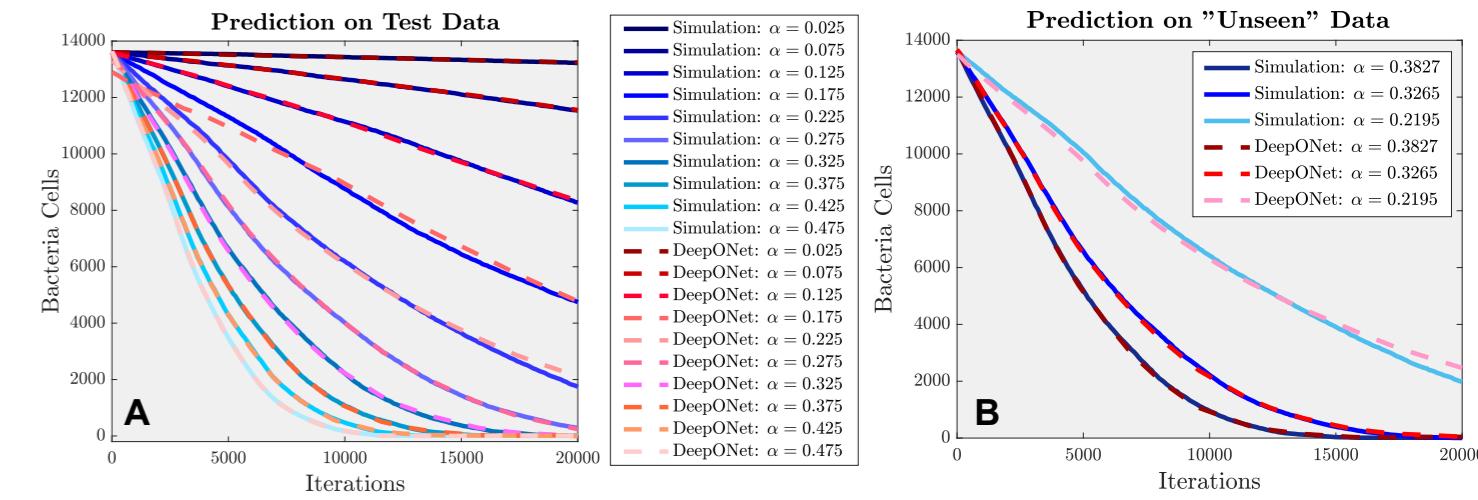
Developed Toolbox



PyLAMDO depends on the Python-LAMMPS interface for automating the simulation + optimization processes.

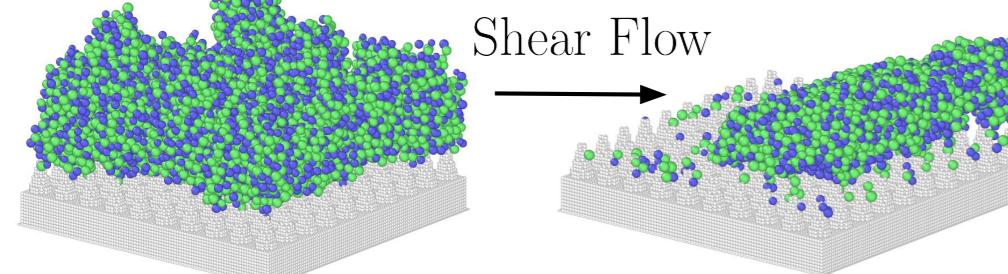
Some Preliminary Results

Inferring biomass from roughness



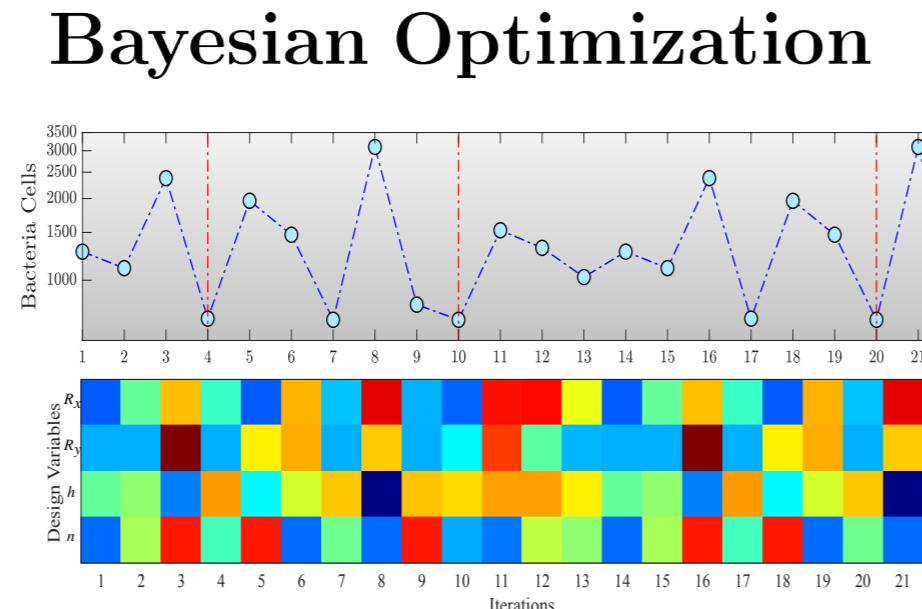
Surrogate model – based designing

Mesoscale Modeling



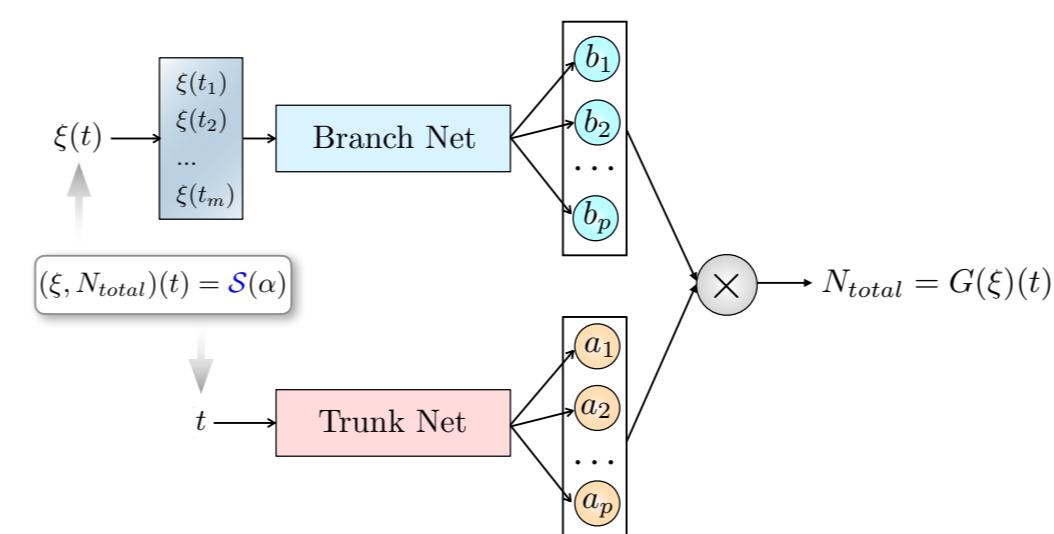
Mesoscale modeling (i.e. DEM) accounts complex physics information.

Methodology

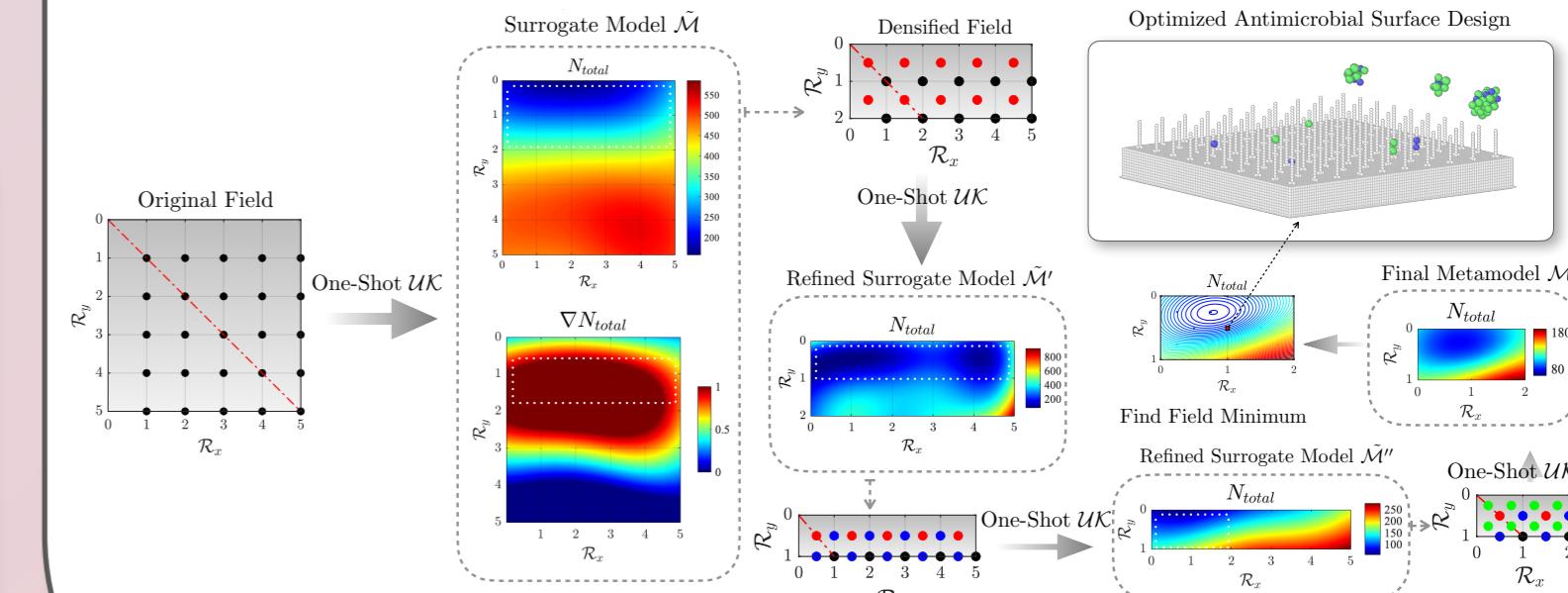


Bayesian optimization is a powerful tool in materials design.

Operator Learning



DeepONet can learning the mapping between functional spaces.



CornellEngineering

