AI for Good + AI for Science

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

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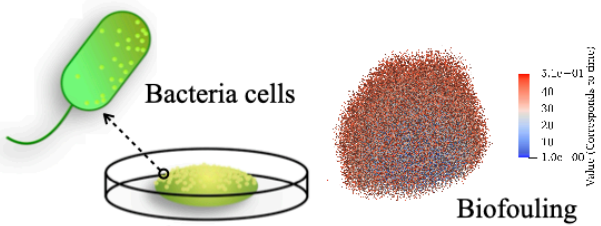
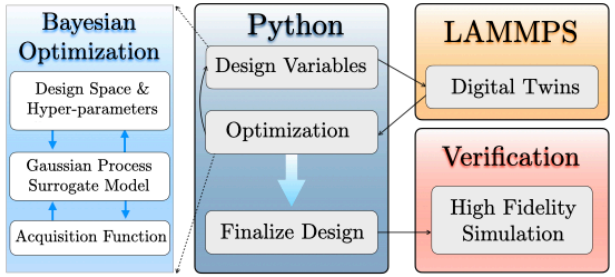
Goal & Objective



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.

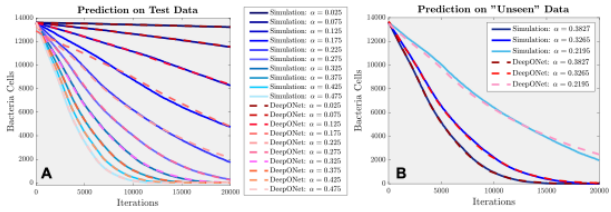
Developed Toolbox



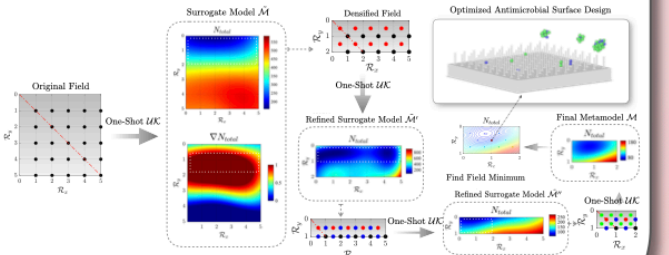
PyLAMDO depends on the Python-LAMMPS interface for automating the simulation + optimization processes.

Some Preliminary Results

Inferring biomass from roughness

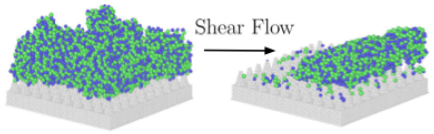


Surrogate model – based designing



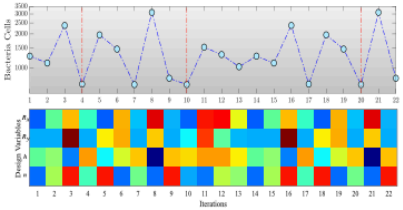
Methodology

Mesoscale Modeling



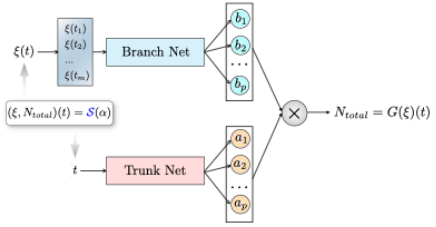
Mesoscale modeling (i.e. DEM) accounts complex physics information.

Bayesian Optimization



Bayesian optimization is a powerful tool in materials design.

Operator Learning



DeepONet can learning the mapping between functional spaces.

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