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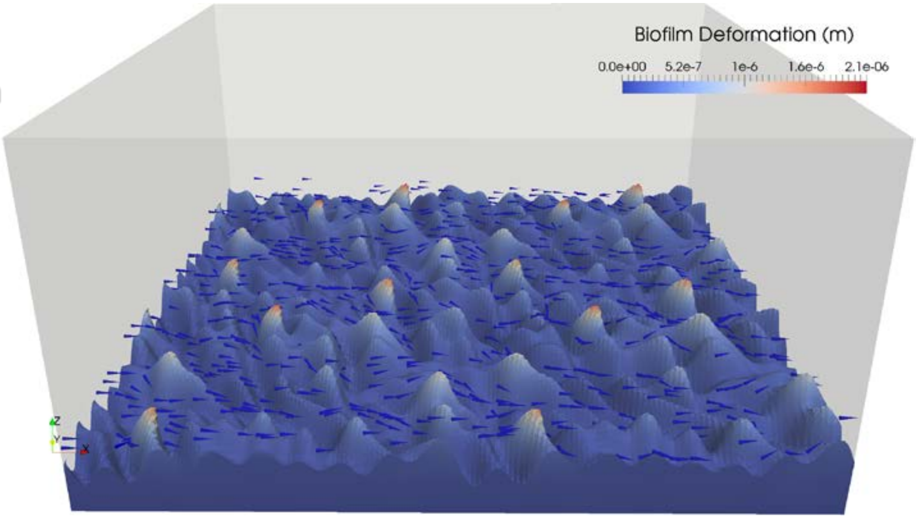
Biology, Chemistry & Health

MULTISCALE MODELING OF BIOFILM DYNAMICS IN DRINKING WATER DISTRIBUTION SYSTEMS: TOWARD PREDICTIVE MODELING OF PATHOGEN OUTBREAKS



Mechanical deformation of a three-dimensional biofilm (in plane dimensions 1mm x 1mm) with multiscale surface roughness subjected to a fluid flow rate of 1m/s. Displacements are highly localized in the biofilm surface peaks suggesting that these areas are most susceptible to fracture.

Research Challenge

The quality of drinking water is a critical public health issue. Thin films made of cells and extracellular polymeric substances that are found ubiquitously on the surfaces of drinking water distribution systems are known to attract, harbor, and hide pathogens from disinfectants and have been linked to pathogenic outbreaks. To fight these outbreaks, we need to improve our understanding of the response of these biological thin films to different types of disinfectants and their susceptibility to fracture under different conditions.

Methods & Codes

We developed a continuum nonequilibrium statistical thermodynamics framework for modelling the nonlinear elasto-plastic response of soft amorphous materials. We implemented this model in a nonlinear finite-deformation framework within the MOOSE platform. To describe biofilm–fluid interactions we use a finite-element code developed by Dr. JaeHyuk Kwack, a member of the Blue Waters team.

Results & Impact

Our results have been pushing the limits of the state-of-the-art in modeling biofilm mechanics. To the best of our knowledge, this is the first three-dimensional model of biofilm—fluid system with complex surface geometry that has ever been created. It is capable of modeling 3D turbulent structures near surface irregularities as well as complex stress patterns that are not apparent from 2D simulations.

Why Blue Waters

The progress accomplished to date would not have been possible without Blue Waters. Each simulation of 3D biofilm—fluid interaction generates tens to hundreds of gigabytes of data and requires 10,000 or more core-hours of runtime.