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

**Allocation:** Exploratory/50 Knh
**PI:** Ahmed Elbanna[1]
**Co-PI:** Helen Nguyen[1]
**Collaborator:** Jaehyuk Kwack[2]

[1]University of Illinois at Urbana-Champaign
[2]National Center of Super Computing Applications, UIUC

## EXECUTIVE SUMMARY

Biofilms are aggregates of cells and extracellular polymeric substances. They are found ubiquitously in both natural and engineered systems, such as on the surfaces of pipes in drinking water distribution systems (DWDS). Biofilms in DWDS have been reported to be capable of attracting and harboring pathogens. In addition, the biofilm matrix may prevent disinfectants from reaching the cells located deep inside the biofilm. As a result, pathogenic microorganisms have been found in DWDS biofilms and have been linked to outbreaks and severe health problems. Understanding the mechanisms of pathogen attachment to biofilms developed in DWDS is of crucial interest to ensure the quality of drinking water and is a critical public health issue. This project contributes to establishing a comprehensive multiscale framework for studying the dynamics of growth and detachment of biofilms in DWDS under different operating conditions by integrating fluid mechanics, solid mechanics, and chemistry to predict pathogenic outbreaks and related public health hazards.

## RESEARCH CHALLENGE

The quality of drinking water is a critical public health issue. The formation and detachment of biofilms in DWDS have been linked to pathogenic outbreaks. Yet, an understanding of the response of biofilms to different types of disinfectants and their susceptibility to fracture under different flow rates and growth environments is still lacking. Several challenges exist, including the absence of a comprehensive constitutive model for the nonlinear and inelastic response of the soft biofilm, the extreme computational demand of the 3D coupled fluid-film simulation, and the numerical challenges associated with meshing the complex biofilm geometry, integration of the tightly coupled partial differential equations governing the chemo-hydro-mechanical response as well as arbitrary growing biofilm fractures in 3D. Progress along these different fronts contributes not only to getting us closer to being able to make quantitative predictions for biofilm response in different operating conditions but also pushes the frontiers of computational science in material modeling and multiphysics simulation.

## METHODS & CODES

Over the past allocation period, we have been able to make fundamental progress in addressing some of these challenges. We have developed a continuum nonequilibrium statistical thermodynamics framework based on the effective temperature approach to model the nonlinear elasto-plastic response of soft amorphous materials. We implemented this material model in a nonlinear finite deformation framework within the MOOSE platform, a finite element framework from Idaho National Lab for multiphysics simulations. MOOSE provides an advanced modular computational infrastructure including the libMesh finite element library and the PETSc solver library. The program requires input of the weak form for partial differential equations to be solved as well as the material model, but it provides a variety of shape functions, stabilization options, and locking control algorithms.

For the bio-film fluid interaction, we used a finite element code for Computational Fluid Dynamics and Fluid-Solid Interaction developed by Dr. JaeHyuk Kwack, who has worked in the Scientific and Engineering Applications Support group at NCSA.

The application code employs a variational multiscale approach for turbulence and nonlinear material modeling; as a result, it provides an optimal computational performance for multiphysics problems that will be investigated through this project. For parallel computation, the code is implemented with the Message-Passing Interface (MPI). As a preprocessing step, numerical meshes are decomposed by the METIS/ParMETIS library. Each MPI process accesses its own decomposed numerical domain (i.e., a series of elements and nodes) and locally computes its residual vectors and tangent matrices. After that, global communications for matrix-vector calculations, assembly process, and residual norm calculations are implemented via the PETSc library. Krylov subspace methods from PETSc and sparse direct matrix solvers (e.g., SuperLU_dist and MUMPS) are employed to solve linear equations with the globally assembled matrices and vectors. The output files are written in VTK file formats and they are post-processed with ParaView.

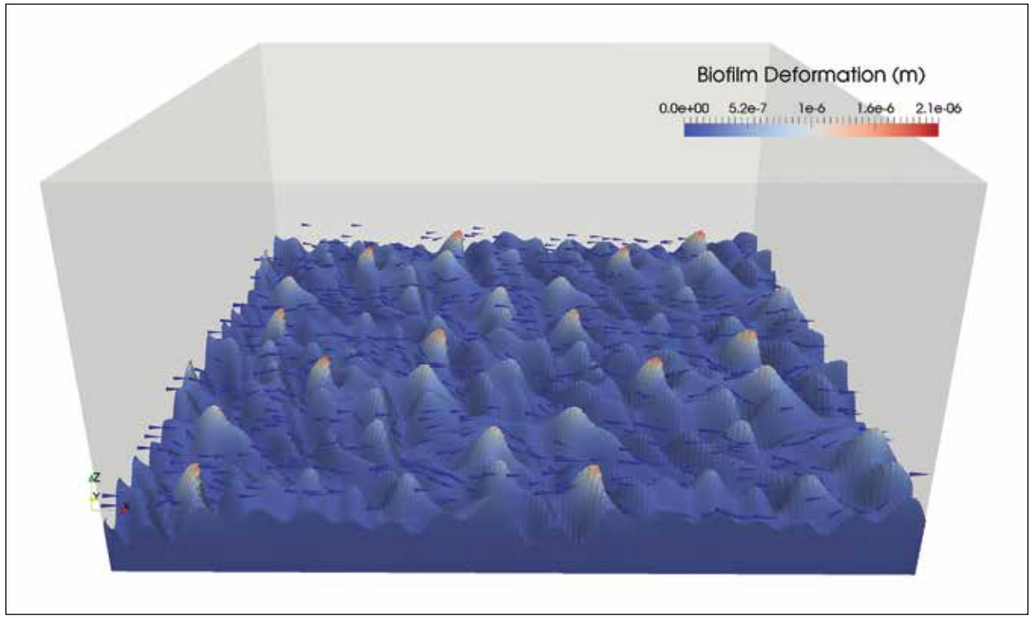


Figure 1: Mechanical deformation of a three-dimensional biofilm (in plane dimensions 1mm x 1mm) with multiscale surface roughness subjected to a fluid flow rate of 1m/s. Displacements are highly localized in the biofilm surface peaks suggesting that these areas are most susceptible to fracture.

## RESULTS & IMPACT

Our results thus far have been pushing the limits of the state of the art in modeling biofilm mechanics. To the best of our knowledge, prior work in the field has been limited to two-dimensional models. We have been able to run full 3D fluid-structure models of biofilm with complex surface geometry. As a result, we can realize complex 3D turbulent structures near surface irregularities as well as complex stress patterns that are not apparent from the 2D simulations. Furthermore, the 3D implementation of the amorphous material model enables us to realize—for the first time—complex strain localization patterns (which will potentially map into complex 3D fracture surfaces) that have not been reported before.

## WHY BLUE WATERS

The progress accomplished so far would not have been possible without Blue Waters. Several of the problems we have tested required 10,000 or more core-hours of runtime and generated tens to hundreds of gigabytes of data per simulation. These resources are not accessible on conventional cluster scales. Furthermore, cloud computing is not suitable for the nature of our problems since any parallelizable discretization of the coupled system of equations of interest would require domain decomposition and efficient communication among processors, making cloud computing out of question.