Network for Computational Nanotechnology - Engineered nanoBIO Node (NCN 1720625)

Rationale and Goals

The design of efficient and safe nanoparticle (NP)-based devices for medical applications (e.g. therapy, sensing) is hindered because we lack a sufficient understanding to link intrinsic NP features and incubation conditions to self-assembled NP clusters, NP-mediated cell and tissue behavior, and ultimately therapeutic response. The Engineered nanoBIO node will develop integrated computational tools that enable researchers to engineer NPs based on the <u>multiscale knowledge</u> of how NPs interface with biological matter at the bioenvironment, cell, and tissue levels. The tools will be <u>community informed, user-tested, and experimentally validated. They</u> will be deployed, supported, and continuously refined on nanoHUB.

Multiscale and Integrated Computational Tools









Extract NP Properties in Bioenvironments

Design Applicationspecific NP Shapes

0.5 – 20 nm

Community Involvement and Outreach ^o User-Informed Spiral Development O Developer Support via Frameworks O nanoBIO Hackathons

Vikram Jadhao, Paul Macklin, Andy Somogyi, James Glazier, Trevor Douglas, Marlon Pierce, Geoffrey Fox Intelligent Systems Engineering, Pervasive Technology Institute, and Department of Chemistry, Indiana University

NP Shape Lab

NP Self-Assembly Lab

Engineer NP Clusters to Interface with Cells

10 – 50 nm

50 – 1000 nm

- ^o Open-sourced on GitHub
- XSEDE Integration for Scalability O Interaction with SGCI to Target MSI





NP-Cell Simulator

Predict NP-mediated Cellular Response

$1 - 100 \,\mu m$

O Summer and All-year REUs ^o Use in Courses; Online Education O Annual Engineered nanoBIO Workshop

