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

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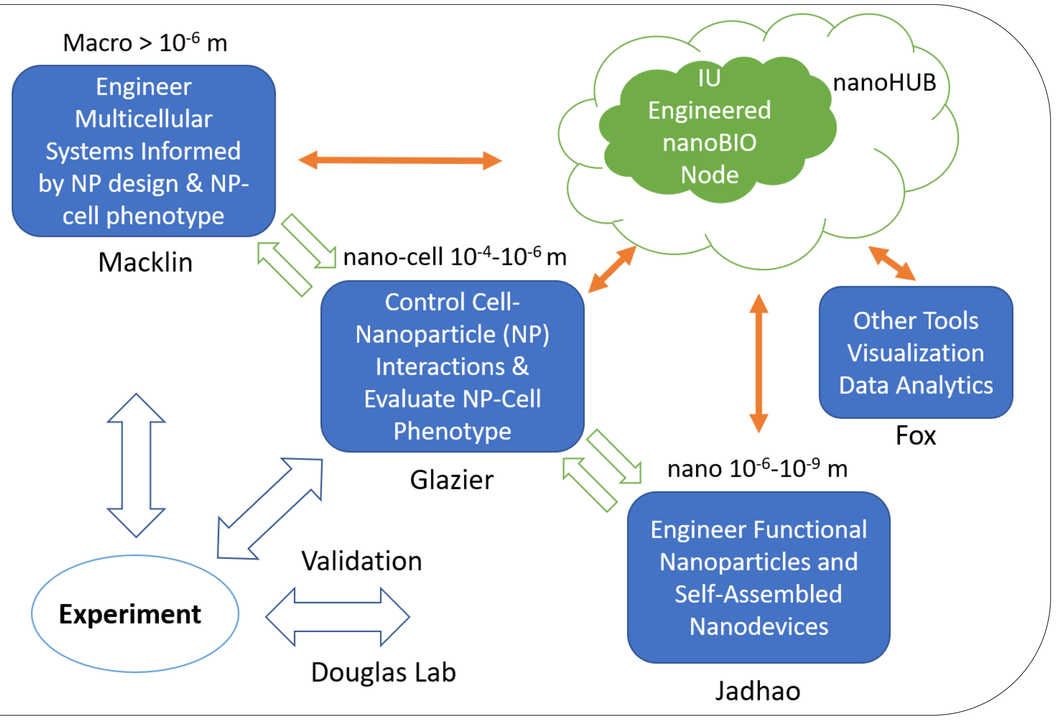
Rationale and Goals

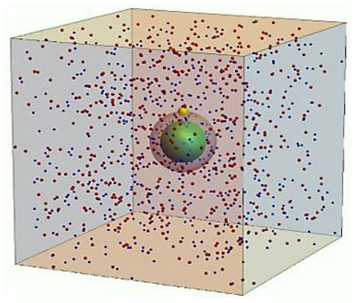
The design of efficient and safe nanoparticle (NP)-based devices for medical applications (e.g. therapy, sensing) is hindered because we lack a sufficient understanding to link intrinsic NP features and incubation conditions to self-assembled NP clusters, NP-mediated cell and tissue behavior, and ultimately therapeutic response.

The **Engineered nanoBIO node** will develop integrated computational tools that enable researchers to engineer NPs based on the multiscale knowledge of how NPs interface with biological matter at the bioenvironment, cell, and tissue levels. The tools will be community informed, user-tested, and experimentally validated. They will be deployed, supported, and continuously refined on **nanoHUB**.



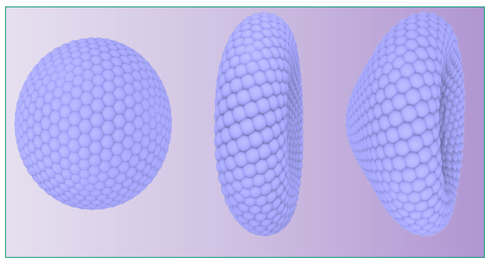
Multiscale and Integrated Computational Tools

NP Characterization Lab



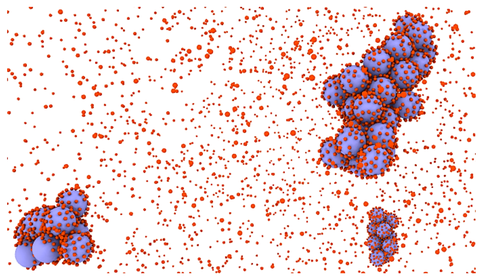
Extract NP Properties in Bioenvironments

NP Shape Lab



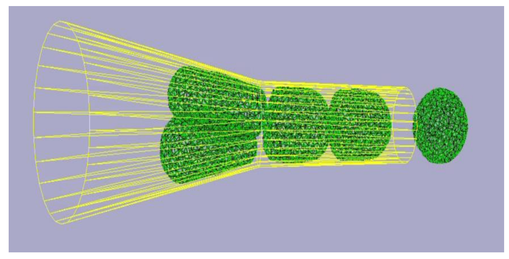
Design Application-specific NP Shapes

NP Self-Assembly Lab



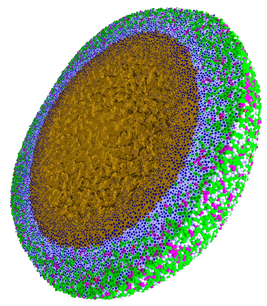
Engineer NP Clusters to Interface with Cells

NP-Cell Simulator



Predict NP-mediated Cellular Response

PhysiCell:nanoBIO



Physics-based Agent Model for 10^6 + Cells

0.5 – 20 nm | **10 – 50 nm** | **50 – 1000 nm** | **1 – 100 μm** | **10 – >1000 μm**

Community Involvement and Outreach

- User-Informed Spiral Development
- Developer Support via Frameworks
- nanoBIO Hackathons
- Open-sourced on GitHub
- XSEDE Integration for Scalability
- Interaction with SGCI to Target MSI
- Summer and All-year REUs
- Use in Courses; Online Education
- Annual **Engineered nanoBIO** Workshop