

Towards a Digital Twin Simulator for Nanomaterial Design in Targeted Drug Delivery and Therapeutics

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DOI: 10.5185/vpoam.2021.03154

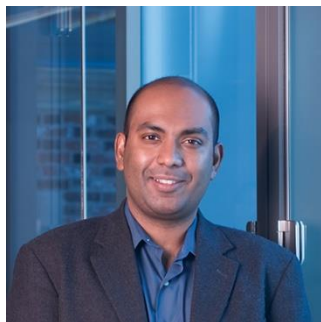
Abstract

The talk will focus on building predictive multiscale models in cell biology and bioengineering using equilibrium and non-equilibrium statistical mechanics, and collaboratively validating such models in *in vitro* physical science-based experiments, *in vivo* in cell culture, and *in vivo* in organisms. The theme will focus on targeted drug delivery using functionalized nanoparticles for nanomedicine and immunotherapy applications. Here we will discuss our efforts in building multiscale models for rigid and flexible nanoparticle targeting to live cells with hydrodynamic, physiological, and molecular factors taken into account. We show how multiscale modeling can help craft a digital twin simulator for enhancing design of nanoparticles. We will also discuss the physical biology of naturally occurring targeted nanoparticles such as exosomes and how they are regulated in the tumor microenvironment to control immune surveillance and response during cancer progression, and how we can harness them in future immunotherapy applications.

Acknowledgements

These works are funded by US NIH, NSF, AFOSR, and EU ERC.

Biography of Presenting Author



Ravi Radhakrishnan has been named Chair of the Department of Bioengineering. Radhakrishnan holds joint appointments in the Department of Bioengineering and the Department of Chemical and Biomolecular Engineering. He is a founding member and the current Director of the Penn Institute for Computational Science, as well as a member of the Penn Physical Sciences in Oncology Center, Institute for Translational Medicine and Therapeutics, and several graduate groups, including Materials Science and Engineering, Genomics and Computational Biology, and Biochemistry and Molecular Biophysics.

In addition to these roles at Penn, Radhakrishnan holds many editorial board positions in the research community, including Nature Publishing's Scientific Reports.

Beyond being a passionate teacher and advocate for his students, Radhakrishnan's research interests lie at the interface of chemical physics and molecular biology. His lab's goal is to provide molecular level and mechanistic characterization of biomolecular and cellular systems and formulate quantitatively accurate microscopic models for predicting the interactions of various therapeutic agents with innate biochemical signaling mechanisms.

Citation of Video Article

Vid. Proc. Adv. Mater., Volume 2, Article ID 2103154 (2021)

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