1163-92-1574 **Yafei Wang*** (wangyafe@iu.edu), 700 N Woodlawn Ave, Bloomington, IN 47408, and **Heber Rocha**, **Randy Heiland** and **Paul Macklin**. *Simulation of drug-loaded nanoparticles on cancer treatment: an agent-based modelling approach.* Preliminary report.

Cancer is a complex systems problem that involves tumor cells and their microenvironment. The application of engineered nanomaterials in medicine for therapy or diagnosis and nanomedicine-biological systems interaction is becoming significant. The mathematical modelling on cancer treatment with nanoparticles (NPs) can be used to explore NPs, tissue, cell, and drug response parameters for a growing tumor, and see for themselves how things could play out for their design choices.

In this work, we propose an agent-based model (with PhysiCell) to investigate the therapeutic designs of cancer treatment with NPs/drug, where NPs internalization, drug release, NPs/drug pass in inheritance and drug effects on tumor cells are explored. Our simulation studies show that drug-loaded nanoparticles have some allowed promising new options for cancer therapy, and the point to the power of using large-scale model exploration to tune and improve therapy. In particular, we introduce a novel tracking of nanoparticle *populations* in each individual cell, allowing better modelling of drug release by internalized nanoparticles, and also providing the capability of modelling the nanotherapy of tumor in multi-generation and long-term therapeutic implications. (Received September 15, 2020)