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Paul Macklin* (macklinp@iu.edu), 4128 Luddy Hall, 700 N Woodlawn Ave, Bloomington, IN 47408. *Exploring agent-based models of complex multicellular cancer systems with HPC.*

Cancer is complex multiscale dynamical system: dysfunctional molecular-scale signaling in cancer cells lead to increased proliferation, decreased death, migration, reduced adhesion, and aberrant metabolism. Cancer cells invade and disrupt local tissues and ultimately metastasize other sites. Chemical and mechanical interactions with other cell types can both promote and inhibit this progression. In this talk, we introduce open source models that combine PDE models of signals and substrates with discrete cell agents to understand complex multicellular cancer systems. We show work to use high performance computing to massively explore a 3-D cancer immunotherapy model, and we show how machine learning can aid model interpretation. (Received September 17, 2019)