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NFsim: A versatile rule-based simulator for complex biological systems MICHAEL SNEDDON, Yale University, MCDB, CBB, JAMES FAEDER, University of Pittsburgh, THIERRY EMONET¹, Yale MCDB and Physics — Traditional methods for biochemical reaction simulation require the enumeration of every possible molecular species and reaction channel, which can be tedious and often impossible for many large or complex systems. We have developed NFsim, a new software platform for exact stochastic simulation of large biochemical reaction networks. By using an agent-based representation of molecules and rules to define interactions, the performance of NFsim is independent of the size of the reaction network. Rates in NFsim can be defined as mathematical or conditional functions of the system to facilitate coarse-graining and general specification of complex models. Here we demonstrate NFsim's novel capabilities with general models of multi-site phosphorylation proteins, receptor signaling and aggregation in the immune system, actin filament assembly, and bacterial chemotaxis signaling.

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