Modeling and Simulation of Discrete Stochastic and Hybrid Systems in GillesPy2

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Stochastic modeling and simulation are valuable tools for understanding biological systems. GillesPy2 is a Python package that allows users to build and simulate stochastic models using an intuitive object-oriented approach. Among the novel features of GillesPy2 is a hybrid algorithm that can simulate models where continuous and deterministic mechanisms are coupled with discrete stochastic processes. The Tau-Hybrid algorithm combines ideas from Gillespie's Tau-leaping algorithm and the random time change representation of stochastic processes. However, maintaining the data structures required by the hybrid algorithm introduces overhead that is not present in specialized code for pure ODE or pure discrete stochastic simulation. We analyze the scaling properties of the Tau-Hybrid algorithm and compare it to ODE and discrete stochastic simulation algorithms. Many aspects of a model influence the efficiency of these algorithms, including the range of time scales, the size of the state vector, and the number of event types (e.g. reactions in a biochemical system). Finally, we discuss the efficiency, and the implementation challenges that arise, when these algorithms are applied to spatially-inhomogeneous models.