Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Biomolecular Network Simulator: Software for Stochastic Simulations of Biomolecular Reaction Networks on Supercomputers[1]
YAROSLAV CHUSHAK, Biotechnology HPC Software Applications Institute, US Army Medical Research and Materiel Command, BRENT FOY, Wright State University, Dayton, OH 45435, JOHN FRAZIER, Air Force Research Laboratory, Wright-Patterson AFB — At the functional level, all biological processes in cells can be represented as a series of biochemical reactions that are stochastic in nature. We have developed a software package called Biomolecular Network Simulator (BNS) that uses a stochastic approach to model and simulate complex biomolecular reaction networks. Two simulation algorithms - the exact Gillespie stochastic simulation algorithm and the approximate adaptive tau-leaping algorithm - are implemented for generating Monte Carlo trajectories that describe the evolution of a system of biochemical reactions. The software uses a combination of MATLAB and C-coded functions and is parallelized with the Message Passing Interface (MPI) library to run on multiprocessor architectures. We will present a brief description of the Biomolecular Network Simulator software along with some examples.

[1]This work was supported by funds provided by the DOD High Performance Computing Modernization Program (HPCMP) and by the Air Force Office of Scientific Research (AFOSR).

Yaroslav Chushak
Biotechnology HPC Software Applications Institute, USAMRMC

Date submitted: 02 Dec 2007 Electronic form version 1.4