

ORNL Titan: Synapse emulating Gromacs simulations of BPTI protein with #atoms  
rp.session.titan-ext1.merzky1.017447.0013: **1024 tasks**; 32 cores/task; 32768 cores;  $\approx 15\text{m}/\text{task}$   
Concurrency of agent queueing, scheduling, scheduling execution, and execution events

