

ORNL Titan: Synapse emulating Gromacs simulations of BPTI protein with #atoms  
rp.session.titan-ext1.merzky1.017447.0018: **2048 tasks**; 32 cores/task; 65536 cores;  $\approx 15\text{m}/\text{task}$   
Concurrency of agent queueing, scheduling, scheduling execution, and execution events

