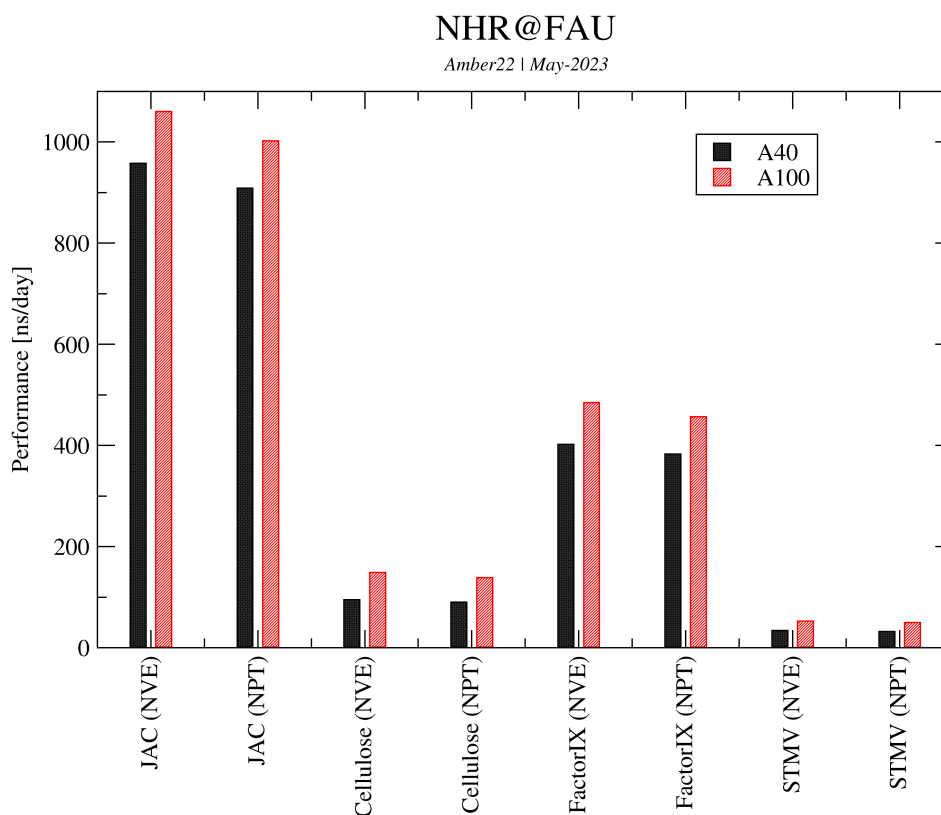


Amber Benchmark Results – NHR@FAU



Overview of Amber benchmarks on ALEX cluster:

System	#Atoms	Ensemble	A40/A100 performance
JAC	23,558	NVE	90.4 %
JAC	23,558	NPT	90.7 %
Cellulose	408,609	NVE	64.0 %
Cellulose	408,609	NPT	65.2 %
FactorIX	90,906	NVE	82.8 %
FactorIX	90,906	NPT	84.0 %
STMV	1,067,095	NVE	64.2 %
STMV	1,067,095	NPT	65.1 %

All simulations were run on Alex with either one A40 or one A100 NVIDIA card; the simulations are restarts, i.e. with atomic coordinates and velocities read in, in different ensembles (NVE or NPT), using a time step of 4 fs via hydrogen mass repartitioning (HMR). Reported are „Standard“ values from the output of the Amber benchmark suite as mean values of eight independent runs of the same molecular system on eight different GPUs of the same type.

Details about the Amber benchmark suite and performance values for different GPUs are available from here: <http://ambermd.org/GPUPerformance.php>