Week 13 - 2020 05 10

What I did

This week I mostly investigated different compiles and run time options. I found very little difference in the different compiles (except that the cpu one is about twice as slow as the k40 gpus, and the v100 one is about twice as fast as the k40 one). Most runtime parameters didn't affect the performance in any significant way.

We cannot use the tune_pme program that tunes the number of pme rank, because this simulation doesn't use any electrostatics.

What I will do

- Grid search parameters + compilers
- investigate single node k40s to try and draw parallels to the dgx that we'll be using.

Current best results

Results

Name	Description	MPI Ranks	NS/day	Nodes	OMP Threads Per Rank
build v1		4	1.288	1	7
build v1		6	1.299	1	4
build v1	-nstlist 100	6	1.299	1	4
build v1	-nstlist 1	6	0.544	1	4
build v1		8	1.316	1	3
build v1	-nstlist 50	12	1.111	1	2
build v1		12	0.688	1	2
build v1	-nstlist 100	12	1.27	1	2
build v2		4	1.343	1	7
build v1	-nstlist 200	12	1.185	1	2
v2		6	1.36	1	4
v2	nsteps 4000	4	1.746	1	7
v2	nsteps 20000	4	1.804	1	7
Build V3→V100		4	2.487	1	7
Build V3→V100		6	2.503	1	4
Build V3→V100	-nstlist 50	4	2.583	1	7
Build V3→V100	-nstlist 150	4	2.603	1	7
Build V3→V100	-nstlist 100	4	2.652	1	7
Build V3→V100	-nstlist 100 -dlb yes	4	2.553	1	7
build v1		8	2.09	2	7

Name	Description	MPI Ranks	NS/day	Nodes	OMP Threads Per Rank
build v1		16	1.85	2	3
build v1		28	2.037	2	2
Build K40 CPU		4	0.606	1	7
Build K40 CPU		6	0.551	1	4
buildV8		4	1.29	1	7
buildV8		6	1.29	1	4

With build script

V3 → On the V100

▼ Build script

```
module load cmake/3.14.3
module load gcc/5.5.0
source /home/mbeukman/intel/2018/parallel_studio_xe_2018.4.057/psxevars.sh
module load cuda/10.0

mkdir build
cd build

cmake ..  -DREGRESSIONTEST_DOWNLOAD=ON \
 -DGMX_SIMD=AVX_256 \
 -DCMAKE_INSTALL_PREFIX=`pwd`/../install \
 -DCMAKE_C_COMPILER=icc -DCMAKE_CXX_COMPILER=icpc \
 -DGMX_MPI=on -DGMX_GPU=on -DGMX_FFT_LIBRARY=mkl 2>&1 | tee cmake.log
make -j28 2>&1 | tee make.log
make check 2>&1 | tee makecheck.log
make install 2>&1 | tee makeinstall.log
```

▼ Run script

```
module load cmake/3.14.3
module load gcc/5.5.0
source /home/mbeukman/intel/2018/parallel_studio_xe_2018.4.057/psxevars.sh
module load cuda/10.0
source ../install/bin/GMXRC
which gmx_mpi

procs=${1:-4}
args=${2:-""}
filename=run-$procs-${args// /-/g}".log"

mpirun -np $procs gmx_mpi mdrun -s lignocellulose-rf.tpr  -gpu_id 0 -nsteps 400 $args  2>&1 | tee logs/$filename
```

Problems

- Nothing seems to change the performance.
- What is nst* mdp options → the messages say that we might want to increase them, but that's in the file we can't access as far as I know.