

# Week 14 - 2020 05 16

What I did

What I will do

Problems

## What I did

This week I just wrote a summary of our gromacs build. I'm not sure what we can do to improve our results. There doesn't seem to be a lot of stuff to change.

Maybe compilers?

I'm looking at a gcc build now. It's probably not better, but you never know.

The gcc build is pretty comparable to the intel one, maybe slightly worse.

## What I will do

Make scripts to run on the pbs cluster.

## Problems

Like in tinker, nothing seems to impact performance to a measurable degree.