Optimisation

Research

Resources

- http://manual.gromacs.org/documentation/2020/release-notes/2019/major/performance.html
- http://manual.gromacs.org/documentation/2020/release-notes/2018/major/performance.html
- http://manual.gromacs.org/documentation/2020/release-notes/2020/major/performance.html
- https://blog.exxactcorp.com/gromacs-2020-highlights/
- https://www.mpibpc.mpg.de/280252/kutzner07talk-optimizing.pdf
- https://www.mpibpc.mpg.de/15381237/kutzner16talk-gromacs.pdf
- **https://www.mpibpc.mpg.de/15230023/Kutzner_2015_JCC_Suppl.pdf** Optimising and stuff
- http://manual.gromacs.org/documentation/current/user-guide/mdrun-performance.html
- http://manual.gromacs.org/documentation/5.1/user-guide/cmdline.html → command line reference
- http://manual.gromacs.org/documentation/5.1/onlinehelp/gmx-mdrun.html

Details

- use `g_tune_pme` to do a kind of grid search for you, with regards to the best pme balance
- Use like `gmx_mpi tune_pme -np 28 -s lol.tpr -launch`
- http://manual.gromacs.org/documentation/2018/onlinehelp/gmx-tune_pme.html

Gromacs is a molecular dynamics code, that uses PME(Particle mesh Ewald). This algorithm does something with electrostatics, and requires all to all processor communication. This is one big hinderance to parallel performance.

-dd is a way to decompose your domain into different size. (Domain decomposition grid, 0 is optimize)

I think it is how the 3d cube is partitioned into cells 0 0 0 is optimized