Exchange

- Exchange matrix with full lattice summation implemented incredibly naively – v expensive
- No truncation or screening as is
- Truncated coulomb operator implemented
- CP2K + libint compiled for testing purposes
- More efficient algorithm identified for screening with M^2 limiting scaling, but ambiguity of how to define codensity center and range

TO DO for exchange (mostly before next time)

- Test vs. cp2k
- Finish implementation of more sensible algorithm with screening – precompute allowed electron pair list with screening
- Faster screening based on fitted analytic form for (ab|ab) integrals
- Implement truncated coulomb operator for higher angular momentum
- Generalize lattice sum
- Integrate with symmetry module to only loop over symmetry-unique atoms, and rest of code

Reflections with hindsight

- Very much enjoy
  - Working as part of a larger project (in some sense more pressure, but also more rewarding)
  - Collaborative aspect
  - Learning new techniques in different area
- Helped by fact that I believe project is worthwhile and important
- Working environment is not the most productive once set up with theory and technical aspects, but since this is often the most time-consuming part, think it is still important to at least start in a communal environment
- C++/fortran interface was a pain, but more importantly limits the readability of the code for fortran-only users and increases their reliance on others.
- Think we should limit the code to C++ only and give the fortran users the more modular isolated projects in the future.
- Existing code -> C++ when working
- Future hackathon should ensure interfaces in place before we start