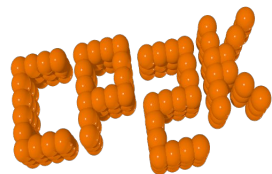# CP2K Developers Meeting

September 29th, 14:00-16:00 2022

CP2K Developers Meeting

1. Introduction
2. Current Issues when running CP2K
3. DeePMD integration (https://github.com/cp2k/cp2k/pull/1620)
   Thomas, will take a look at it
4. PRACE Benchmark Suite
5. RPA and SOS-MP2 gradients (Frederick Stein)
6. CP2K Verification Project (Thomas Kühne/Matthias Krack)
7. CP2K Roadmap paper (https://arxiv.org/abs/2209.12747, https://arxiv.org/abs/2205.14741)
8. Low-scaling GW for 2D semiconductors (Jan Wilhelm)
9. NewtonX (Anna Hehn)
10. CP2K Release (all)
11. CP2K-related Events (all)
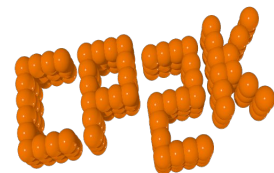
Introduction
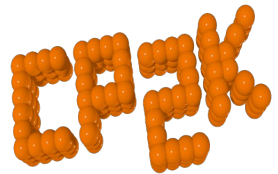
Current issues when running cp2k

- CP2K on CSCS systems seems to trigger some bug in mpi. It is difficult to fully exclude bugs in cp2k either. It affects users running the latest version of cp2k as well as the official version.
  (no open ticket right now, so unclear, all tests successful)
- DBCSR was particularly unstable when compiled with GPU support on ORNL and NERSC systems (both cray systems).
  (unclear, maybe related to openblas on POWER?)
  (A100 kernels: maybe merge with V100 kernels, because V100 tunings work well on A100, too.)

PRACE Benchmark Suite

Should we try to swap the LS-DFT benchmark from the PRACE Benchmark Suite for one that targets the tensor code?

That code powers many of our recent additions, including GW and the various RI methods. As a bonus, it would also give vendors a new opportunity for contributing optimizations.

Differences:

- block sizes (skinny and tall and much more different)
- MPI communication in tensor lib instead of in matrix multiplication

Todo Ole/Hans: confirm maximal number of benchmarks

Other options: QM/MM (GEEP, FIST), SIRIUS?, COSMA

Proposal:

- make preliminary benchmark like above @Ole
- gather experience and insight into scaling and behaviour @all

Status:
Ole contacted (former) people, situation of PRACE unclear (EURO-HPC, BREXIT,...), but benchmarks are still very important but rules unclear
Goal: three scalable benchmarks but should also work on a few nodes
Suggestion: drop DFT-LS
RPA: has benchmark (already in use for LUMI)
GW: Jan Wilhelm (smallest calculation would already require ~32 nodes)

RPA and SOS-MP2 gradients (Frederick Stein)

Gradients of correlated methods are available with all relevant kernels (MP2, RPA, SOS-MP2, high-scaling and low-scaling)

all of them are GPU accelerated (SpLA, COSMA, DBT)

High-scaling RPA/SOS-MP2

- on Daint not enough GPU memory for reasonable performance (128 H_2O) with COSMA (use libsci instead)
- on LUMI probably less memory issues (WIP)

Maybe: prioritize GPU memory usage issue

Alfio is open to answer some questions and share his experience with optimizing COSMA

Maybe: high-level questionare in toolchain (scale, performance, GPU-setup) and better documentation/explanation

Next Steps: Brainstorming list of typical performance/configuration problems

Interface between NewtonX and CP2K

Revised code for original NewtonX, includes by default orbital derivative couplings, Baeck-An couplings and local diabatization

2nd NewtonX code on Gitlab (FIXME add link)

Libra-CP2K interface by Prof. Akimov (https://github.com/AkimovLab/Project_Libra_CP2K)

Juerg Hutter

- xTB bug (periodic part of coulomb, better but not final yet)
- ongoing master thesis: Frank-Condon-factors for excitations (to be finished start of next year)
- new functionals: Density-corrected SCAN-functional (gradients and stress tensors)

Ole: Type annotations are recommended (mypy --strict, https://mypy.readthedocs.io/en/stable/index.html)

Questions

Q: Are there any plans to allow assignment/utilization of GPU acceleration through the Fortran/C++ interface of CP2K? (This question is still unanswered)

Q: Support for Apple and other platforms and OSes?

● Apple M1 isn't working right now (DBT-tests are failing, OpenMP-related)
● Workaround: Linux native on M1
● Minimal example (reproducer needed)
● Ole: Setup ARM test on GCP

Multi-gpu-support:

● Test in Dashboard

Todo: Tests on HPC systems

CP2K-related events:

Ideas: Paderborn

- QM/MM with together with Gromacs
- Post-HF in CP2K (EXX, RPA, GW,...)