CP2K Developers Meeting

August 18th, 2023 14:00-16:00 CEST
1. Announcements of Meetings
2. Current Development Efforts (all)
3. Current Development Efforts: New Documentation (Ole Schütt)
5. ….
6. Software Support CASUS/HZDR (Frederick Stein)
7. ….
8. Current Issues when running CP2K (all)
9. Feature Deprecation (all)
10. CP2K Release (all)
11. CP2K-related Events (all)
Announcements of meetings

Did Github Discussions work well? How did you learn about the meeting?

Shortcomings:
- everything is public (slide access,...)
Current Development Efforts

What are you currently working on or planning to work on?

- **Jan Wilhelm:**
  - improve scaling of low-scaling periodic GW, trade 3-center integrals for lesser memory demands (also other low-scaling approaches could profit from this step)
  - SOC in pseudopotentials now in CP2K

- **Augustin Bussy**
  - RI-HFX with k-point sampling, now benchmarking for efficiency and accuracy, also works with ADMM

- **Dorothea Golze**
  - interface to GreenX
  - Help with toolchain part appreciated: Ole

- **Bo Thomsen:**
  - interface between PIMD and CP2K, working on GPU assignment
  
Multi-GPU (Ole Schütt)

- Multi-GPU = multiple GPUs per CPU
- Prime example LUMI
- Essentially a new architecture:
  - Data has to remain on GPU.
  - GPU-to-GPU communication is key.
  - More workloads onto GPU (Amdahl's law).
- Bad News: Descent support will take 5+ years at current pace
- Good News: NVIDIA Grace-Hopper returns to 1 GPU per CPU ratio
cuSOLVERMp (Ole Schütt)

- New Eigensolver from Nvidia ([documentation](#)).
- Supports multi-node and multi-GPU.
- Experimental [support](#) shipped with CP2K 2023.2 release.
- Optimization for largish matrices (50k) is ongoing.
- Very slow (and still a bit buggy) for small matrices:
  - unclear how to handle different sized matrices (cusolvermp, scalapack, distribution?)
  - maybe do the same as for ELPA
Modernization of Grid Code (Ole Schütt)

- Collocate and integrate already done.
- Let's modernize everything in-between too.
- Goal: Keep grids on the GPU.
- Goal: Support CPUs with 100+ cores.
- Need to apply MPI strategies to OpenMP threads.
- Could leverage new features in FFTW.

Call to arms!

- Frederick Stein is planning to work on it
Current Development (Thomas Kühne)

- efforts together with Stefanie Gräfe
- use i-pi protocol: forces, calculated with their code
- CP2K for MD propagation
- maybe as an interface to ML-potentials
## Current Development Efforts: HFX

1. **Restructuring of HFX component:**
   a. dynamic load balancing instead of static distribution with support for preferences of MPI ranks for certain quartet classes (currently with master-client system, possibly change to work-stealing)

2. **Accelerator implementations**

<table>
<thead>
<tr>
<th>device class</th>
<th>person</th>
<th>primitive cartesian ERIs</th>
<th>primitive spherical ERIs</th>
<th>compression</th>
<th>contracted ERIs</th>
<th>Hamiltonian on device</th>
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</thead>
<tbody>
<tr>
<td>CPU</td>
<td>libint, libcint, (libintx)</td>
<td>exists</td>
<td></td>
<td>exists</td>
<td>planned to be used</td>
<td>-</td>
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<tr>
<td>CUDA</td>
<td>Marcello Puligheddu, Matt Watkins</td>
<td>done</td>
<td>done</td>
<td></td>
<td>planned</td>
<td>planned</td>
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<tr>
<td>HIP</td>
<td>Lukas Mazur</td>
<td>in progress</td>
<td>in progress</td>
<td>in progress</td>
<td>planned</td>
<td>planned</td>
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<tr>
<td>Intel GPU (OpenMP, OpenCl, SyCL)</td>
<td>anyone interested in trying? maybe SYCLomatic? HIP compiler for Intel</td>
<td></td>
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<td></td>
<td></td>
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<tr>
<td>Intel FPGA</td>
<td>Xin Wu</td>
<td>done</td>
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<tr>
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<tr>
<td>Xilinx AI Engines</td>
<td>Johannes Menzel</td>
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<td></td>
<td>planned</td>
<td>unclear</td>
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</tbody>
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Current Development Efforts: SOC (Jan Wilhelm)

- benchmarking effort necessary compared to other implementations
Software Support CASUS/HZDR (Frederick Stein)

- Since August Professional Support at CASUS/HZDR (Görlitz, Germany)
- Support and Implementation of Features, Events
- Check [https://github.com/users/fstein93/projects/3/views/1](https://github.com/users/fstein93/projects/3/views/1) for an overview of possible projects

- Current ideas: Optimization of Grid operations (LibXC, Splines, PW/RS-grids, FFTs, …)

- Open positions: 1-2 developers (DBCSR/DBM/DBT, k-points/symmetry, …)

Mail: f.stein@hzdr.de
Revamp Documentation (Ole Schütt)

- Move user docs out of the wiki...
- Use git and pull requests instead.
- Use Markdown and Sphinx for formatting.
- Use *The documentation system*:
  - **Reference**: Done.
  - **Howtos**: Migrate [cp2k.org/howto](http://cp2k.org/howto).
  - **Tutorials**: Migrate [cp2k.org/exercises:common](http://cp2k.org/exercises:common).
  - **Explanation**: Write / curate textbook style articles.
A GUI for CP2K (Ole Schütt)

- Hypothesis: A lot of science is limited by usability.
- Bad News: Usability improvements are not publishable.
- Goal: Make CP2K self-teachable
- Goal: Make CP2K users more productive
- Working title "CP2K-Lab"
- GUI runs in the browser
- Calculations run in the cloud
- Funding: Ideally freemium, realistically charity
Current Issues when Running CP2K

- Matthias Krack: Intel compiler 2021.8.0 and 22.2 and a newer one issue in grid code
  - wait and hope for ifx
Feature Deprecation

Idea:

1. Mark a feature/functionality as to be deprecated. Write large warning message with instruction to notify cp2k-community (e.g. via issue) if feature is still used.
2. Remove feature/functionality some versions later.

Thoughts:

- mention which last version had the deprecated feature
- keyword importance (expert) or deprecation filtering

What do you think?

Planned removals:

- old TDDFT code (Hutter)

Suggestions for possible removals:

- maybe old fft code (check wavelet solver and dependencies)
- maybe internal xc-functionals (probably not all, performance considerations, LDA-PADE)
- maybe single-precision on the high-level data structures
CP2K-Release
CP2K-related events:

Ideas:

- Paderborn+CASUS/HZDR:
  - ~Q1/24: Gromacs & CP2K on QM/MM (school with tutorial, 3-4 days in person)
  - ~Q3/24: Post-DFT/HF in CP2K: ADMM, RI, RPA,... (workshop with talks, 1-2 days virtual)