CP2K Developers Meeting

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Ongoing Developments and News from E-CAM Workshop

- k-points
  - State of development
  - Integration of spglib
  - Integration of SeekPath
- RI-Methods
  - RI with overlap metric
  - Single function expansion: collocate and integrate
- Pseudopotentials
- E-CAM Workshop
  - POP CoE: OmpSs, Performance testing
  - Open Path Sampling (OPS): Python API
  - E-Cam: easybuild, singularity, JUBE

k-points

- Full grid k-point is working
- time-reversible reduction (to be committed)
- DKH/ZORA (to be committed)
- Optimize and improve load balancing (99% of time)
  `do_general_diag_kp`
  `rskp_transform`
  `dbcsr_desymmetrize_deep`
  `dbcsr_complete_redistribute`

sgplib

- `atztogo.github.io/spglib/index.html`
- Version 1.9.9
- Features
  Find symmetry operations
  Identify space-group type, Wyckoff position assignment
  Find a primitive cell
  Search irreducible k-points
- CP2K Documentation needed
- k-point reduction, symmetry matrices and non primitive cells

Band Structure

SeeK-path: the k-path finder and visualizer

`http://materialscloud.org/tools/seekpath`

- CP2K input format or use a support input format
- Transfer output of symmetry point labels and high-symmetry path to CP2K input

RI-Methods with Overlap Metric

$$(\alpha\beta \mid \gamma\delta) = \sum_{PQRS} (\alpha\beta P)\,(PQ)^{-1}\,(Q \mid R)\,(RS)^{-1}\,(S\gamma\delta)$$

Applications

- $\mathcal{O}(N^3)$ RPA and G0W0
- HFX at Γ point
- HFX for k-points
- TDDFT: kernel

Overlap RI-Methods for GGA DFT

Global version of LRIGPW

$$\rho(r) = \sum_R a_R \chi_R(r)$$

$$N = \mathbf{n}^T \cdot \mathbf{a}$$

$$\mathbf{R}_{uv} = (\chi u, \chi v)$$

$$\mathbf{T}_{\alpha\beta u} = (\varphi_\alpha, \varphi_\beta, \chi u)$$

$$\mathbf{Ra} = (\mathbf{P} \cdot \mathbf{T}) - \frac{\lambda}{2}\mathbf{n}$$

$$\lambda = \frac{2\mathbf{n}^T\mathbf{R}^{-1}(\mathbf{P} \cdot \mathbf{T}) - 2N}{\mathbf{n}^T\mathbf{R}^{-1}\mathbf{n}}$$

Collocation and Integration

- Full replication of **a** vector
- Direct collocation and integration on PW grids
- Parallelization within MPI tasks
  Junks of grid points build tasks -> no dependencies
- Communication free (except replication of **a** and result of integration)

Pseudopotentials

- Make ECP library available in CP2K
  Approximation in nonlocal form (accuracy?)
  GAPW/GPW ?

- Nonlocal and semilocal PP from the UPF library (Quantum-Espresso)
  Numerical functions fit to Gaussians
  Approximation in nonlocal form

- Mostly for test and benchmark purposes (not performance).

E-CAM Workshop

- Barcelona 6/7 July 2017
  Extreme-scale state-of-the-art workshop

- POP CoE
  Performance analysis (3 day workshop in December)
  Loop parallism -> task parallelism (OmpSs)

- Open Path Sampling (OPS) `openpathsampling.org/`
  Jan-Hendrik Prinz, David W.H. Swenson, John Chodera, Peter Bolhuis (Amsterdam)
  `CP2K` engine planned

Alan O'Cais (E-CAM Jülich)

- EasyBuild
  EasyBuild is a software build and installation framework that allows you to manage (scientific) software on High Performance Computing (HPC) systems in an efficient way.
  `http://easybuild.readthedocs.org`
  CP2K builds available

- Singularity `http://singularity.lbl.gov/`
  Singularity enables users to have full control of their environment. Singularity containers can be used to package entire scientific workflows, software and libraries, and even data.

- JuBE (from Jülich)
  Automatic Testing and Performance Measurement System