Erlangen Regional Computing Center

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

HPC – Café Talk

Services for Quantum Mechanics and related users

HPC Services, RRZE

High Performance Computing

Tobias Klöffel

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

- Newest member of HPC group
- Chemistry (MoWi) studies / PhD
  @ Computer Chemistry Center (B. Meyer)
- Experience with
  - Quantum Espresso
  - CPMD
  - ORCA
  - OpenMPI / IntelMPI
  - ScaLapack / Lapack / ELPA / MPI / OpenMP
- Interested in
  - VASP
  - CP2k
  - … (what ever you use)

What we can do for you?

- Provide software packages as modules
- Benchmarking
- Coding (KONWHIR)
- Performance monitoring
- Things we are not yet aware of!

QE Parallelization

- Do not use Hyperthreading, always use 20 tasks per node
- OpenMPI (3.1) mpirun --report-bindings --bind-to core --map-by ppr:1:core
- Compile with ELPA support
- Use –ndiag for systems #bands > 500
- Use K-Point parallelization –npools
- -npools should be a divisor of #k-points
- -npools must be a divisor of #MPI tasks
- Rule of thumb: 1 k-point / node
- Use gamma point approximation if possible
  - ⇒ KPOINTS GAMMA

- Other options:
  - -nimage, -nband, -ntg

VASP Parallelization

- NCORE = 10
- #band / 8
- … benchmarking!

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Questions!?

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https://hpc.fau.de

High Performance Computing