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FÜR MATHEMATIK, INFORMATIK
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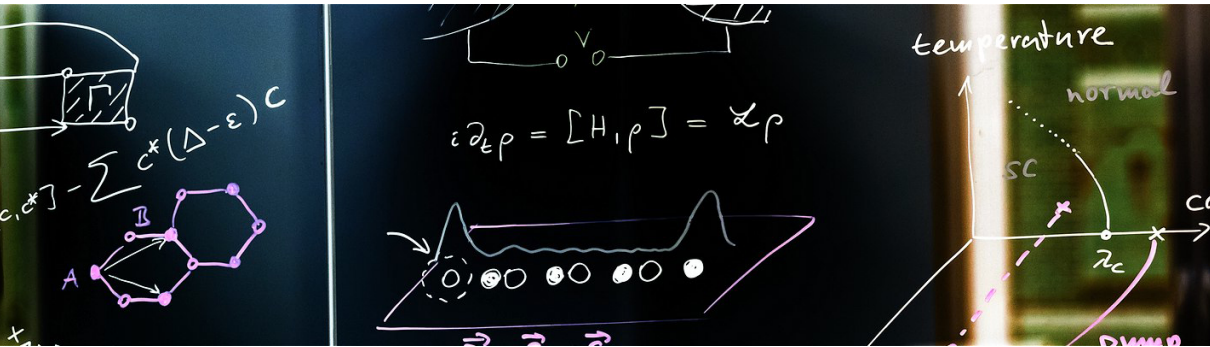

Tjark Sievers – I. Institute of Theoretical Physics 13th July 2022

Optimization of the Quantum Espresso Density Functional Theory Code for parallel execution on the PHYSnet-Cluster

Motivation

- Computing resources are limited, both in time and memory available
- This means: work has to be distributed efficiently among multiple processors
- Codes like QUANTUM ESPRESSO offer capabilities to tune how exactly the workload is distributed

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I aim to answer some questions:

- How big is the effect of good/bad parallelization?
- How does hardware topology play into it? (PHYSnet: 20 cores per node)
- How can one find good parallelization parameters?

Speedup

How much faster can a problem be solved with N processors instead of one?

$$S := \frac{T_1}{T_N}$$

with serial runtime T_1, runtime on N cores T_N

Ideal case: every processor needs the same time

$$T_N = \frac{T_1}{N} \implies S = \frac{T_1}{\frac{T_1}{N}} = N$$

Amdahl's Law

In reality: several factors limiting parallelization: communication between processors, startup time, algorithmic limitations

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Simple model given by Amdahl's law

$$S = \frac{T_1}{T_N} = \frac{1}{s + \frac{1-s}{N}}$$

with s the part of the calculation which cannot be perfectly parallelized

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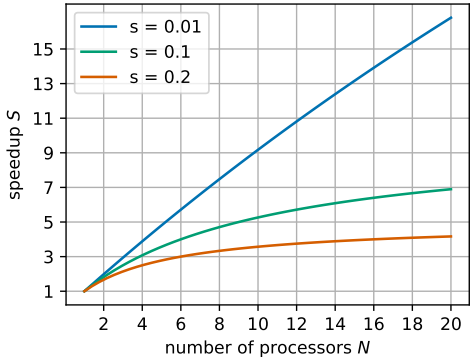
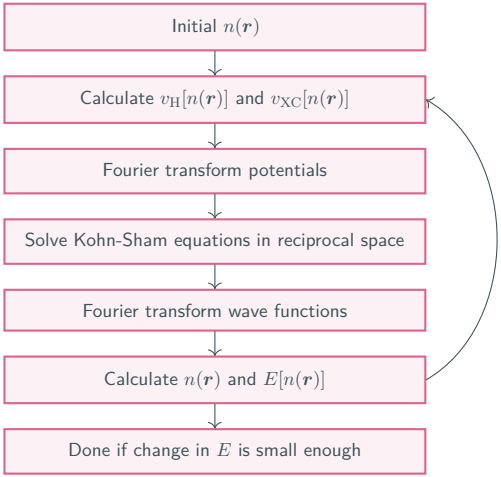


- upper bound for speedup given by $1/s$
- smaller s: closer to $S = N$ for more processors

Solving the Kohn-Sham equations



Basis set for periodic systems: plane waves

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{G}} e^{i(\boldsymbol{k}+\boldsymbol{G})\boldsymbol{r}}$$

Multiple ways to parallelize:

- distributing grids in real/reciprocal space (R/G parallelization)
- solve Kohn-Sham equations for different k-points separately (k-point parallelization)

Parallelization parameters

QUANTUM ESPRESSO has the argument `nk`: determines number of processors pools the available processors are split into (for k-point parallelization)
$\rightsquigarrow$ different partition of the processors, depending on the total number of processors

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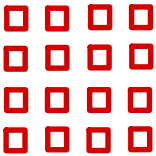
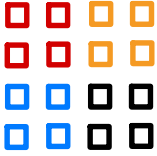


`nk 4`



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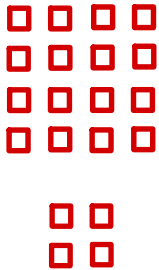

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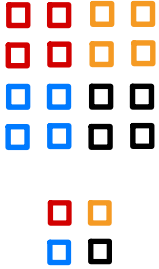

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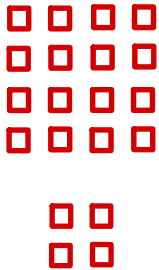

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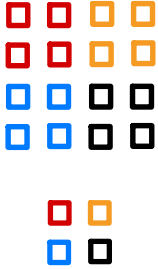
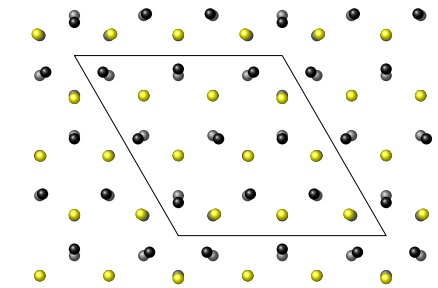
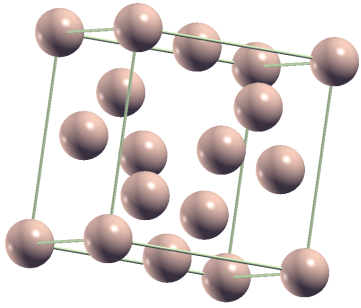


$\rightsquigarrow$ use size of the resulting pools for comparison, not the parameter `nk`

Examined systems

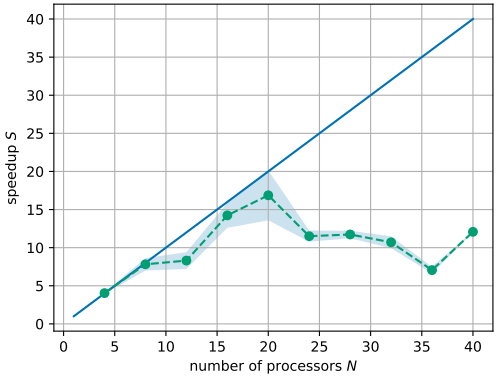


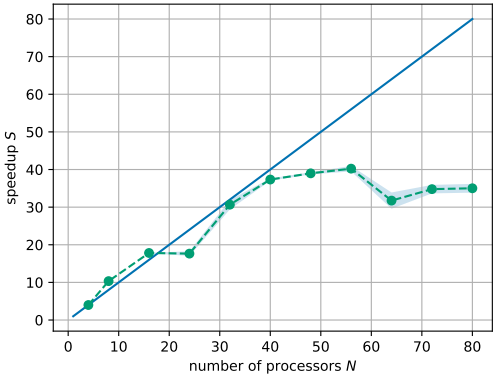
Monolayer Tantalum Disulfide (TaS_2)
light gray: symmetric structure
dark gray/yellow: charge density wave phase



Silicon

Electronic structure
No k-point parallelization

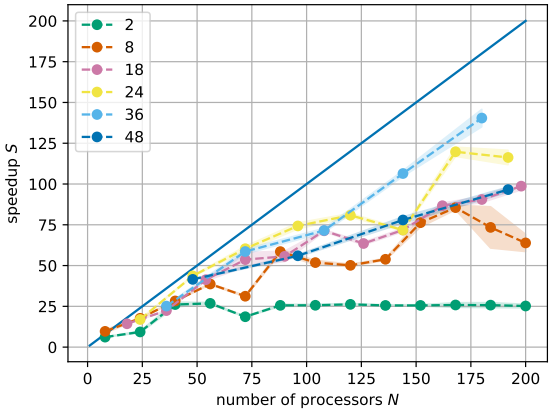




- OpenMPI/gcc compilers
- decline in speedup after 20 processors

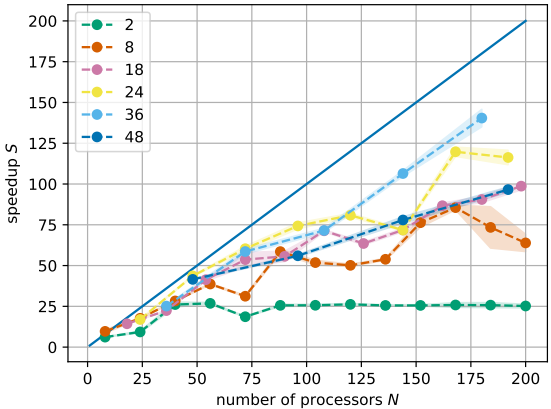
- Intel compilers
- ideal speedup for up to 40 processors

Electronic structure
k-point parallelization

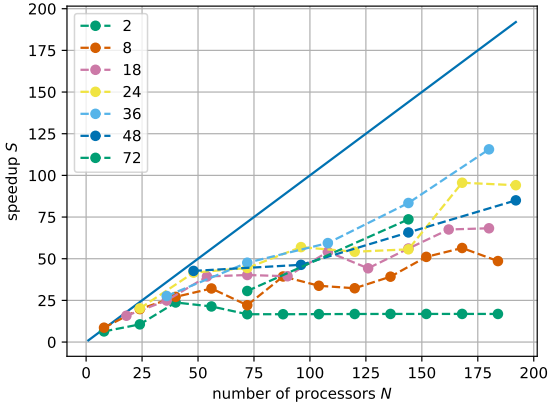


- pool size 36 scales best
- consistent with the results of the benchmark without k-point parallelization

Electronic structure
k-point parallelization



PHYSnet



HLRN

Phonons
Preliminaries & k-point parallelization

DFPT: again a set of equations to be solved self-consistently

Multiple ways to parallelize:

- R/G parallelization
- k-point parallelization
- separate calculations for different phonon wave vectors q (image parallelization)

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- k-point parallelization
- separate calculations for different phonon wave vectors q (image parallelization)

Phonon calculations at $q = 0$
Two pool sizes tested, both on 180 processors:

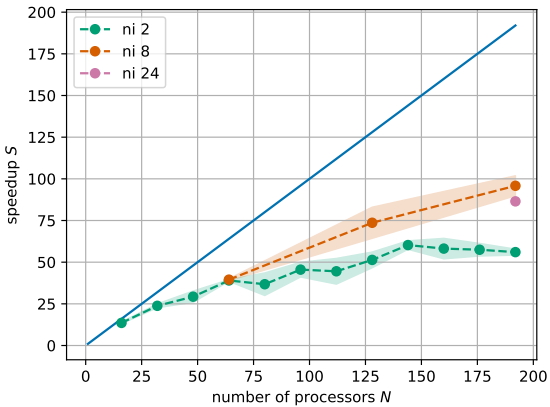
- pool size 18: 3044 min
- pool size 36: 2020 min

Difference already after first phonon mode:

- pool size 18: 2832.1 s
- pool size 36: 2183.3 s

$\rightsquigarrow$ optimal pool size translates over modules

Phonon calculations
Image parallelization



- benchmark run on bulk silicon
- for that system: pool size 8 performed best

⇝ benchmark with combinations of `ni` and `nk` with resulting pool size of 8

- linear scaling continues when using more images

Conclusion

- goal of this thesis: examine how QUANTUM ESPRESSO calculations parallelize, measured by speedup

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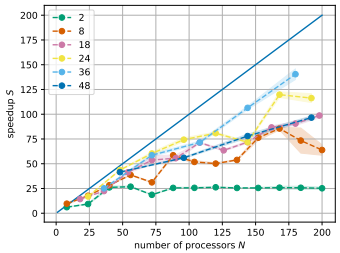
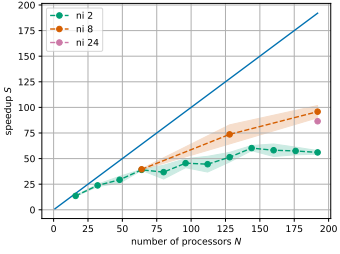
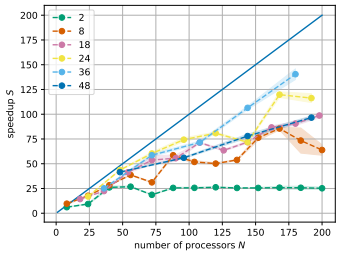
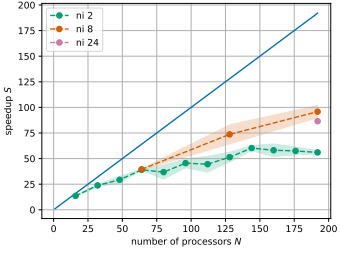




Conclusion

- goal of this thesis: examine how QUANTUM ESPRESSO calculations parallelize, measured by speedup
- right choice of parallelization parameters has a significant impact on the runtime of calculations with QUANTUM ESPRESSO
- good choice of parameters translates between the two modules examined and between different compute clusters





Additional slides

k point parallelization: Memory

Electronic structure calculations on TaS_2, 180 processors

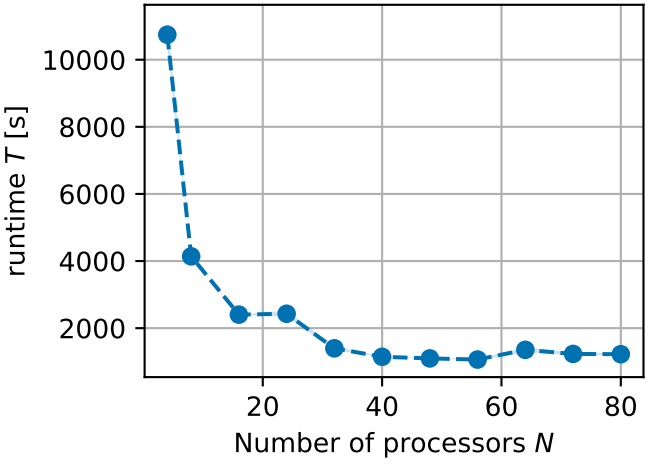
pool size 18:

- estimated max dynamical RAM per process $>$ 178.04 MB
- estimated total dynamical RAM $>$ 28.67 GB

pool size 36:

- estimated max dynamical RAM per process $>$ 103.76 MB
- estimated total dynamical RAM $>$ 17.07 GB

Electronic structure calculations



Amdahl's Law: limitations

- no distinction between different limiting factors: e.g. communication limits parallelization with some dependence on N

$\rightsquigarrow$ serial part s gives no information about what could be improved