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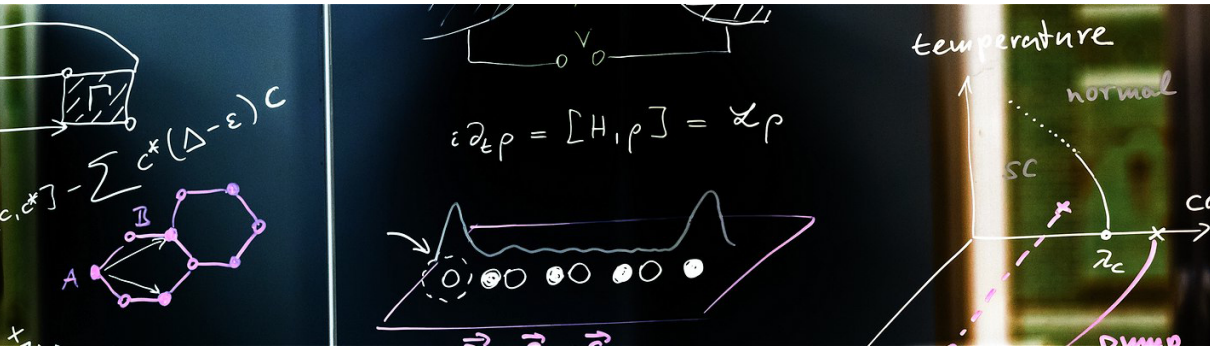
FAKULTÄT
FÜR MATHEMATIK, INFORMATIK
UND NATURWISSENSCHAFTEN



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

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?

$$S := \frac{T_1}{T_N} \tag{1}$$

with serial runtime T_1, runtime on N cores T_N

Ideal case: every processor needs the same time

$$T_N = \frac{T_1}{N} \implies S = \frac{T_1}{\frac{T_1}{N}} = N \tag{2}$$

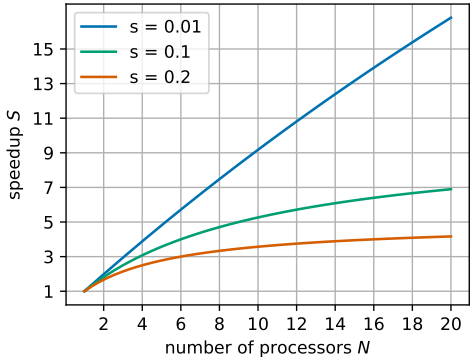
Amdahl's Law

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

Simple model given by Amdahl's law

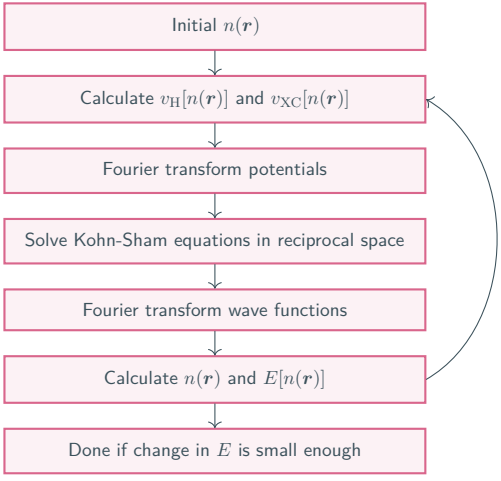
$$S = \frac{T_1}{T_N} = \frac{1}{s + \frac{1-s}{N}} \qquad (3)$$

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



- 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

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{G}} e^{i(\boldsymbol{k}+\boldsymbol{G})\boldsymbol{r}} \tag{4}$$

Multiple ways to parallelize:

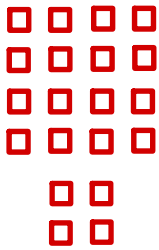
- distributing grids in real/reciprocal space (R/G parallelization)
- solve Kohn-Sham equations for different k-points separately (k-point parallelization)
- (additionally in DFPT) separate calculations for different phonon wave vectors q (image parallelization)

Parallelization parameters

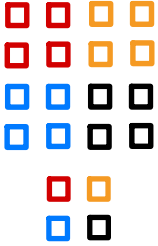
QUANTUM ESPRESSO has the argument `nk`: determines number of processors pools the available processors are split into (for k-point parallelization)

$\Longrightarrow$ different partition of the processors, depending on the total number of processors

no k point parallelization

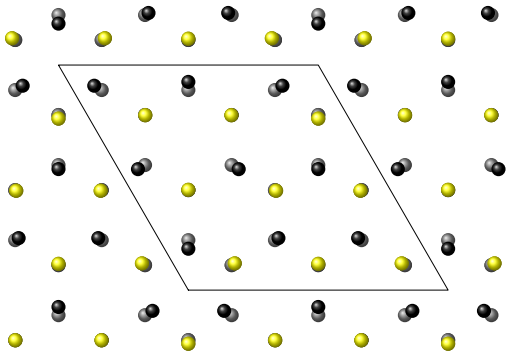


`nk 4`



Use size of the resulting pools for comparison, not the parameter `nk`

Examined system

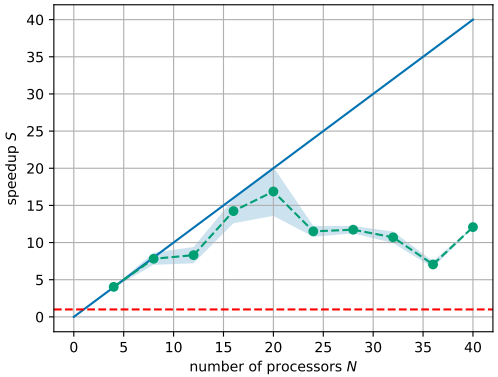


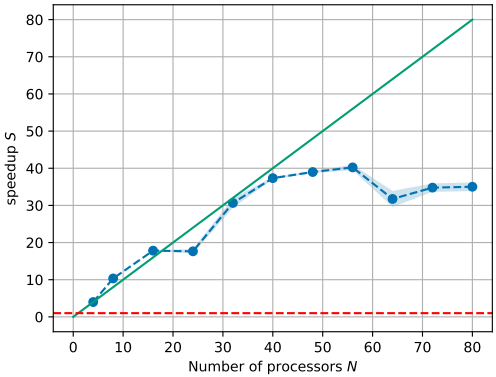
light gray: symmetric structure
dark gray/yellow: cdw structure

Monolayer Tantalum Disulfide (TaS_2) in a 3×3 charge density wave

Benchmarking electronic structure calculations

No k-point parallelization

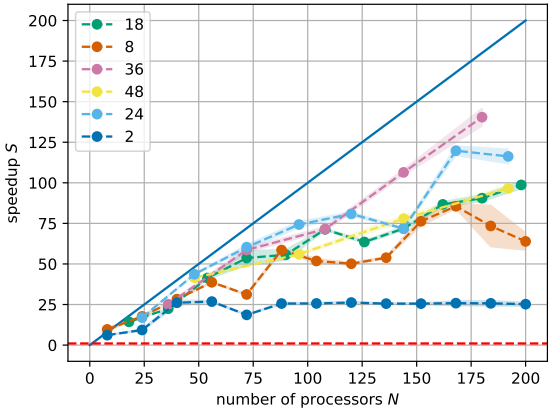




- OpenMPI/gcc compilers
- decline in speedup after 20 processors

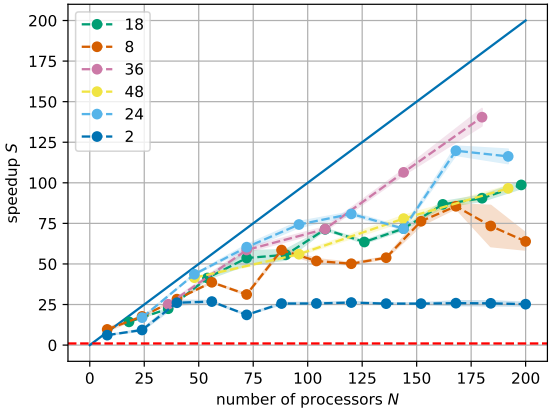
- Intel compilers
- ideal speedup for up to 40 processors

k-point parallelization

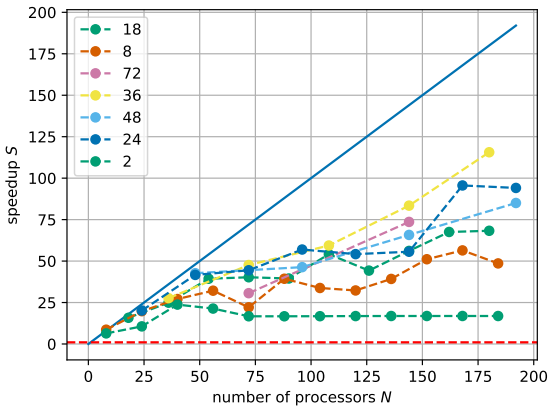


- pool size 36 scales best
- consistent with the results of the benchmark without k-point parallelization

k-point parallelization



PHYSnet



HLRN

Benchmarking phonon calculations

k-point parallelization

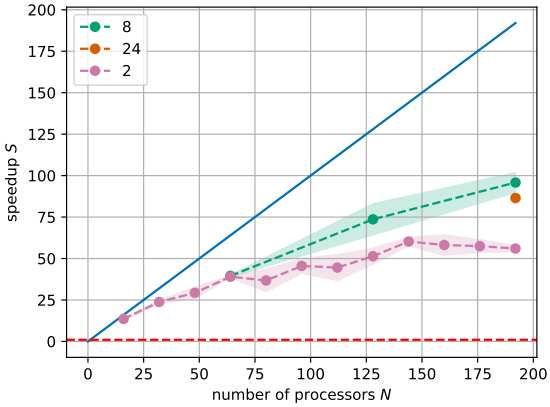
Two pool sizes tested, both on 180 processors:

- 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

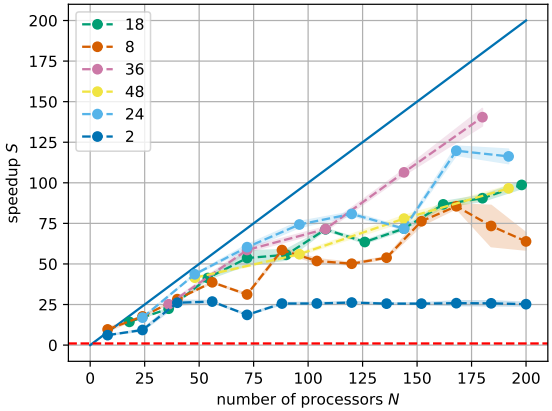
Image parallelization



- benchmark run on bulk silicon
- different combinations of `ni` (different colors in the plot) and `nk` with resulting pool size of 8
- linear scaling continues when using more images

Conclusion

- 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 as well as between different compute clusters



PHYSnet

Additional slides

k point parallelization: Memory

Electronic structure calculations on TaS_2, 180 processors

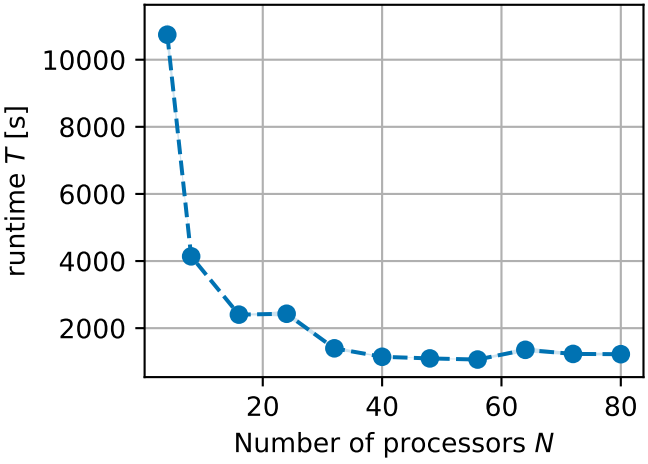
pool size 18:

- 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



Linear Algebra parallelization

Amdahl's Law

Simple model given by Amdahl's law:

- split serial time into serial part s and perfectly parallelizable part p:

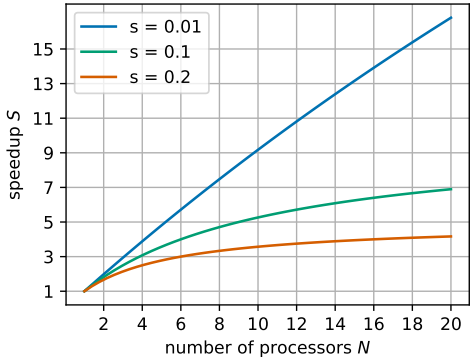
$$T_1 = s + p = 1 \tag{5}$$

- execution time on N processors:

$$T_N = s + \frac{p}{N} \tag{6}$$

- speedup:

$$S = \frac{T_1}{T_N} = \frac{1}{s + \frac{p}{N}} = \frac{1}{s + \frac{1-s}{N}} \tag{7}$$



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