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BMBF Projekt 01IH15001

Porting the ELPA library to the KNL architecture

MIC Programming Workshop @ LRZ

Dr. Andreas Marek

together with

Dr. Hermann Lederer, Dr. Pavel Kus, Dr. Lorenz Hüdepohl

MPCDF Max Planck Computing & Data Facility

Outline

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- What is the ELPA libary
- A roofline model for KNL
- Writing AVX-512 kernels
- Going to many nodes
- KNL experiences
- Conclusions

The ELPA library: Eigenvalue solvers for Petaflop applications

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- ELPA is a high-performance library for the massively parallel solution of dense, symmetric (hermetian) eigenvalue problems

- replacement for Scalapack routines (pdsyevd, pzheevd, pdsyevr, pzheevr)

- widespread used, e.g. in electronic structure codes

- opensouce (see https://elpa.mpcdf.mpg.de)

- available with many linux distributions (Debian, Fedora, Suse etc..)

- supports a large variety of platforms (X86, X86_64, OpenPower, BG P/Q, GPUs, KNL)

- achieved already 0.3 PFLOPS/s on 294k cores (BG/P FZJ Juelich in 2011)

The ELPA library: Eigenvalue solvers for Petaflop applications

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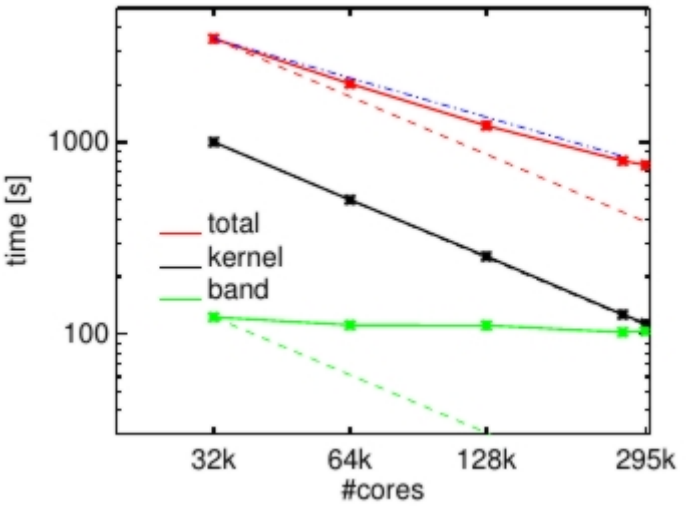
=> used in many HPC centers worldwide (Juelich, Cineca, ORNL, LLNL …)

=> nowadays used in most material science codes (FHI-aims, Quantum Esspresso, VASP, OpenMX…)

=> Intel is interested in integrating ELPA in it`s MKL library



The ELPA Library - Scalable Parallel Eigenvalue Solutions for Electronic Structure Theory and Computational Science. A. Marek, V. Blum, R. Johanni, V. Havu, B. Lang, T. Auckenthaler, A. Heinecke, H.-J. Bungartz, and H. Lederer, The Journal of Physics: Condensed Matter 26, 213201 (2014).

Parallel solution of partial symmetric eigenvalue problems from electronic structure calculations. T. Auckenthaler, V. Blum, H.-J. Bungartz, T. Huckle, R. Johanni, L. Krämer, B. Lang, H. Lederer, and P. R. Willems: Parallel Computing 37, 783-794 (2011).

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The ELPA library: Eigenvalue solvers for Petaflop applications

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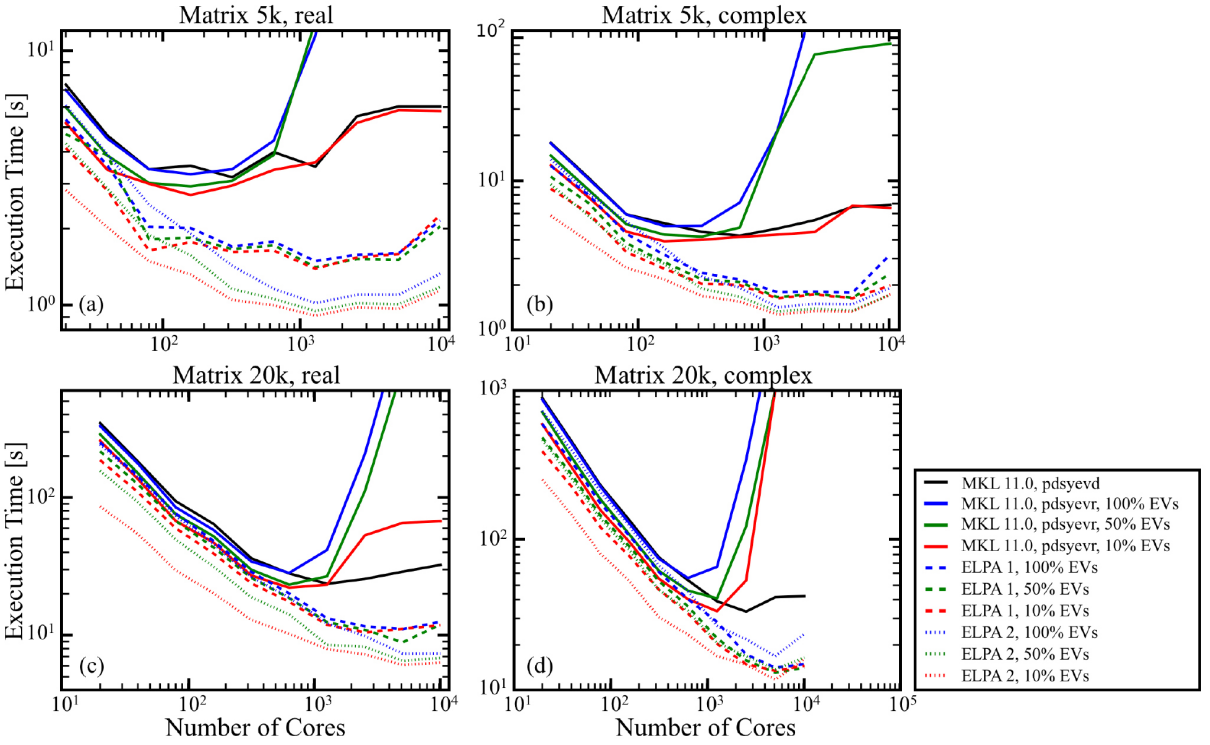

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Development of the ELPA library

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- The development of the ELPA library started under the lead of MPCDF in 2008; it has been funded by a BMBF project 01IH08007 from Dec. 2008- Nov. 2011
- ELPA is maintained and developed at MPCDF
- Since Feb. 2016 a new BMBF project 01IH15001 is funding the latest developments of ELPA (including the porting to KNL)

The algorithm in a nutshell - I

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1. step: - transformation of matrix to banded matrix
- store information for later back-transform

The algorithm in a nutshell - II

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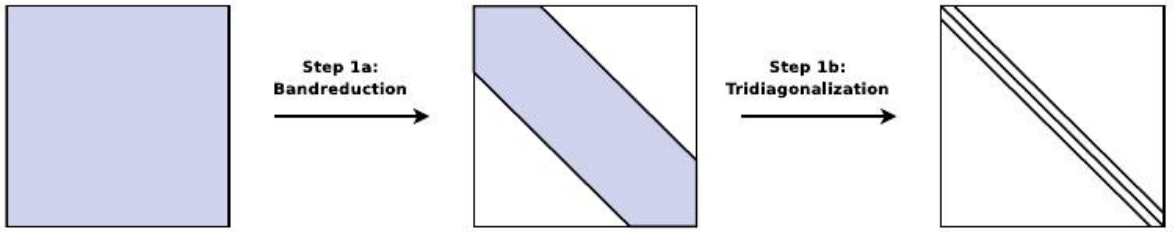

2. step: - transformation to tridiagonal matrix
- store information for later back-transform

The algorithm in a nutshell - III

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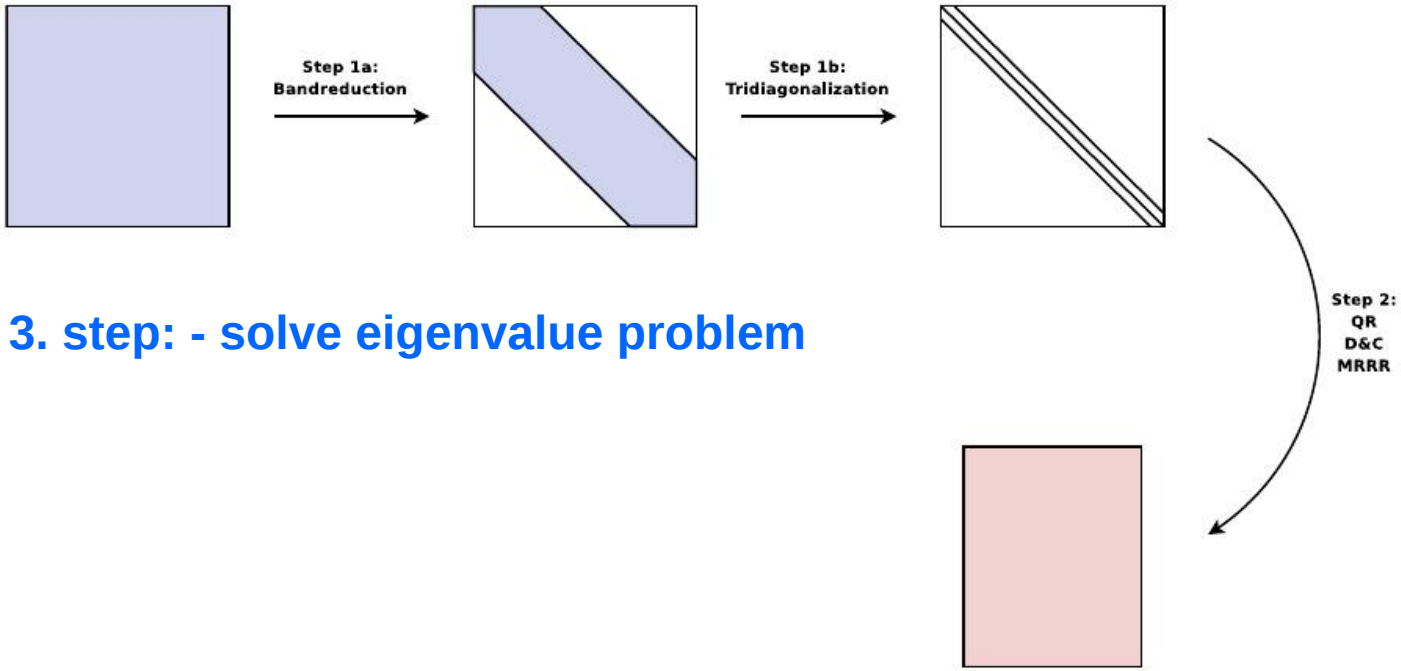

3. step: - solve eigenvalue problem

The algorithm in a nutshell - IV

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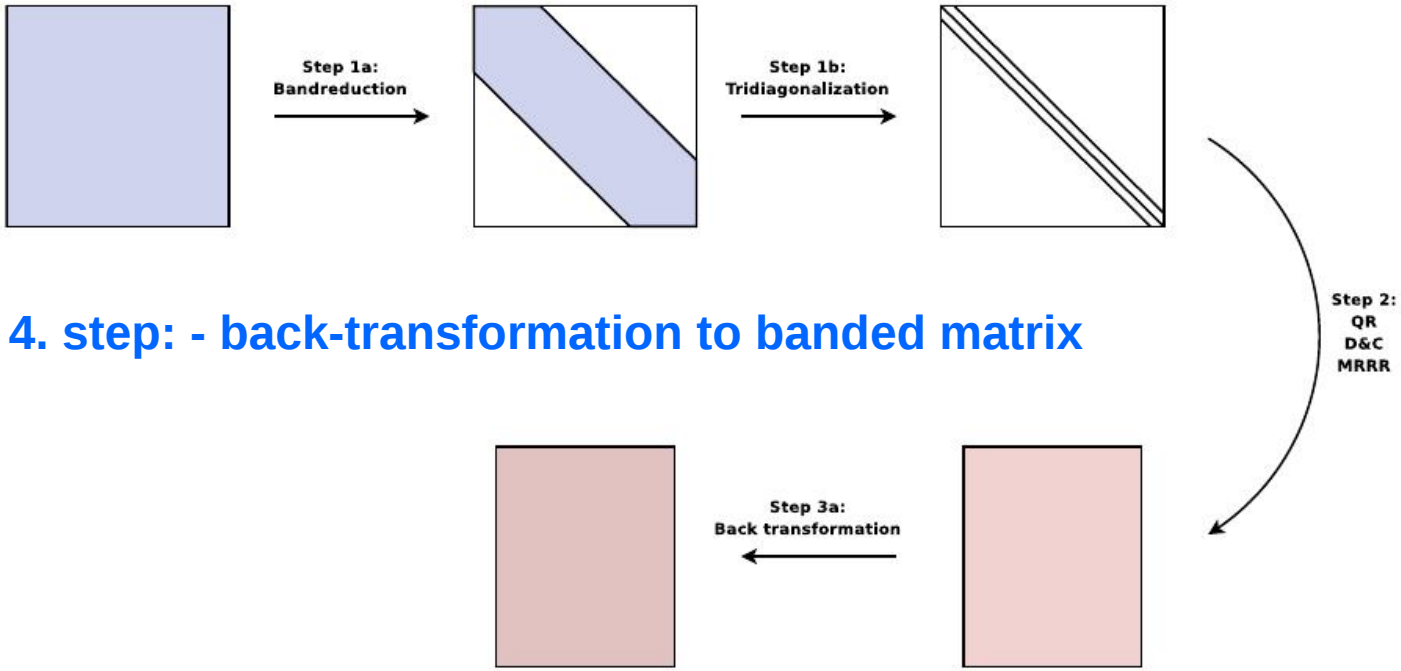

4. step: - back-transformation to banded matrix

The algorithm in a nutshell - V

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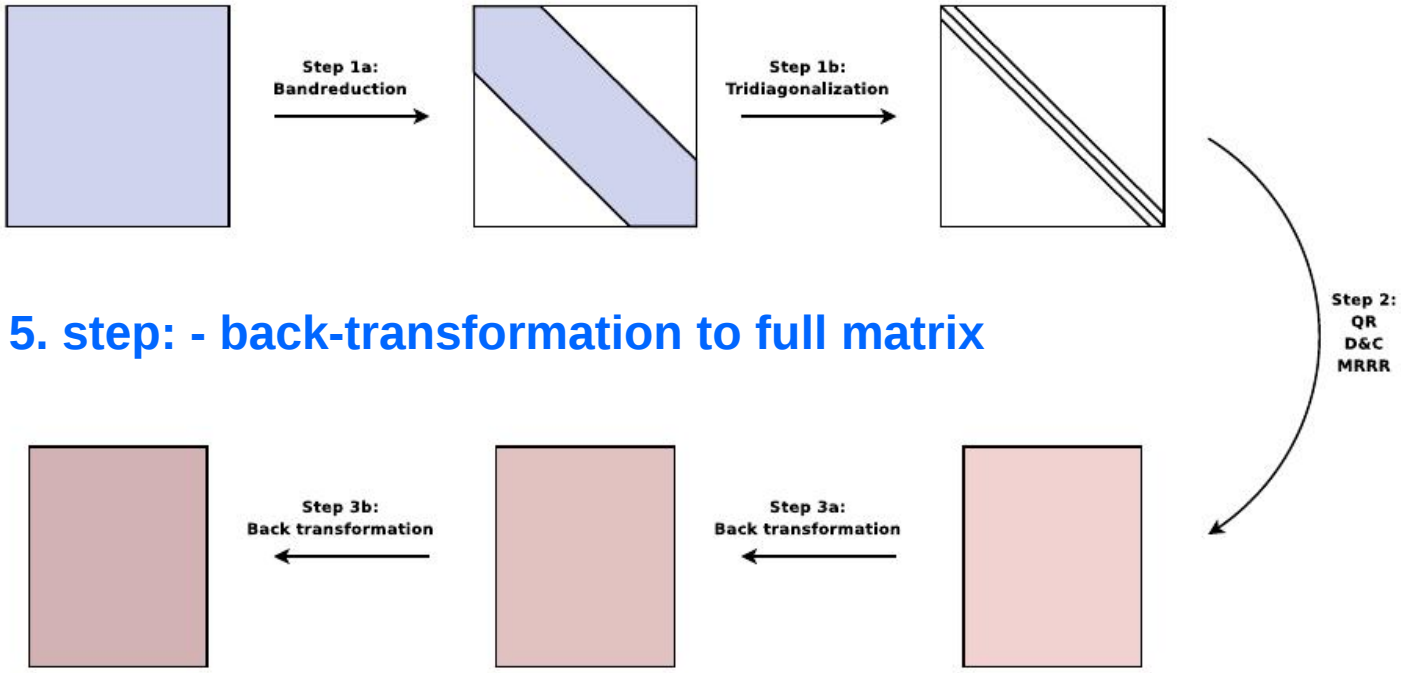

5. step: - back-transformation to full matrix

The algorithm in a nutshell - VI

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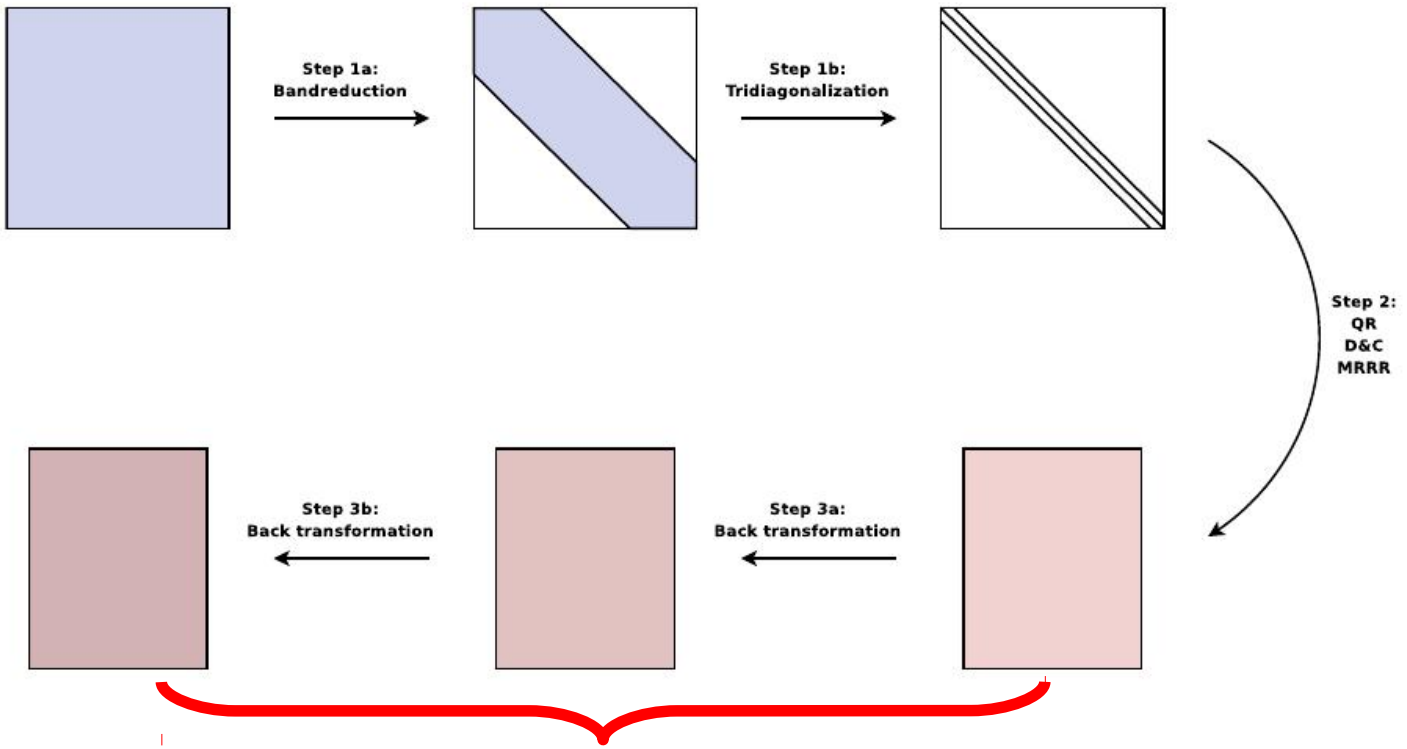

The backtransformation is computationally expensive and relies on optimized kernels

Estimates on possible KNL performance - I

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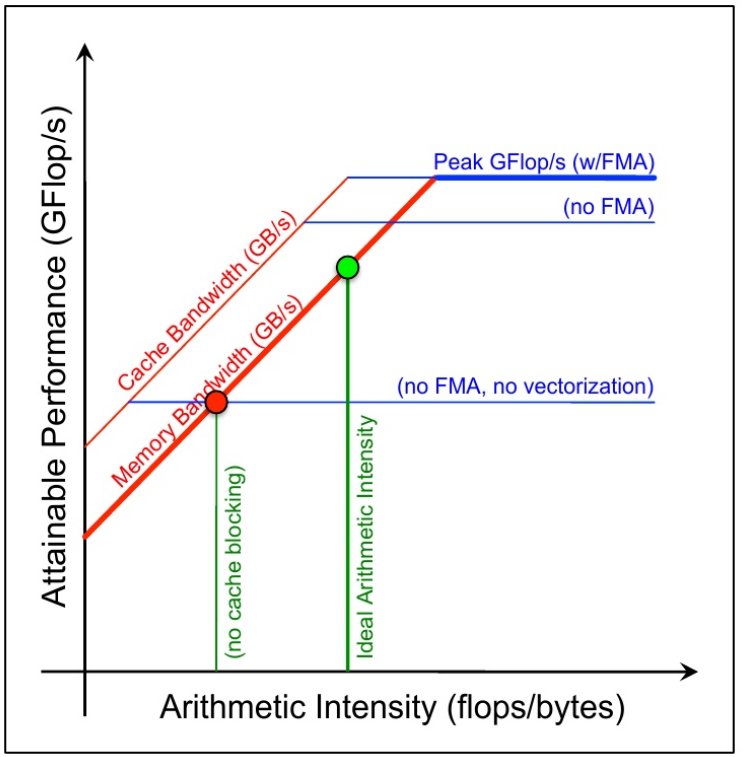
- **Prior to porting ELPA (and especially judging the performance) we want to have a feeling on what you can expect/get on a new architecture**

  => roofline model is helpful

  very nice work of NERSC in the NESAP project

Typical arithmetic intensities in BLAS routines:

BLAS Level 2 (Matrix-Vector): ~O(1)
BLAS Level 3 (Matrix-Matrix): ~O(n)



„Applying the roofline performance model to the Intel Xeon Phi Knights Landing processor“, D. Doerfler, J. Deslippe, S. Williams, L. Oliker, B. Cook, T. Kurth, M. Lobet, T. Malas, J.-L. Vay, and H. Vincenti, Lawrence Berkley National Laboratory

Estimates on possible KNL performance - II

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BLAS Level 2 (Matrix-Vextor): ~O(1)
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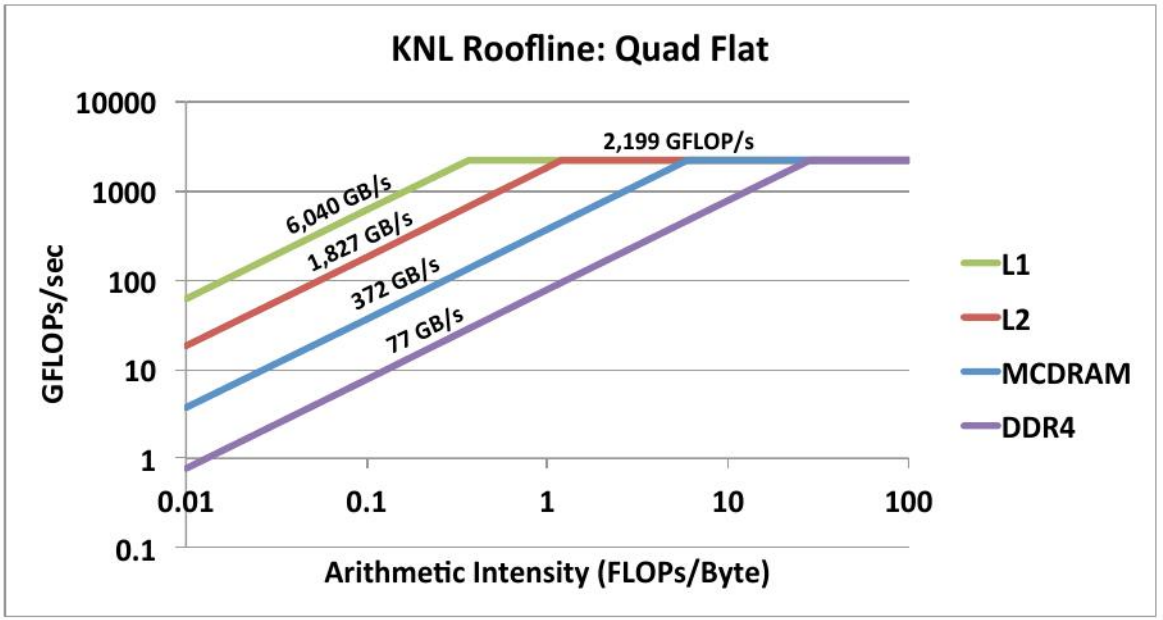

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Porting the kernels to AVX-512 - using Intel`s SDE

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- we have used Intel`s „Software Development Emulator“ (http://software.intel.com/en-us/articles/intel-software-development-emulator) on a standard Haswell node to develop the AVX-512 kernels

- together with Intel`s AVX intrinsic guide (https://software.intel.com/sites/landingpage/IntrinsicsGuide)

Porting the kernels to AVX-512 - using Intel`s SDE

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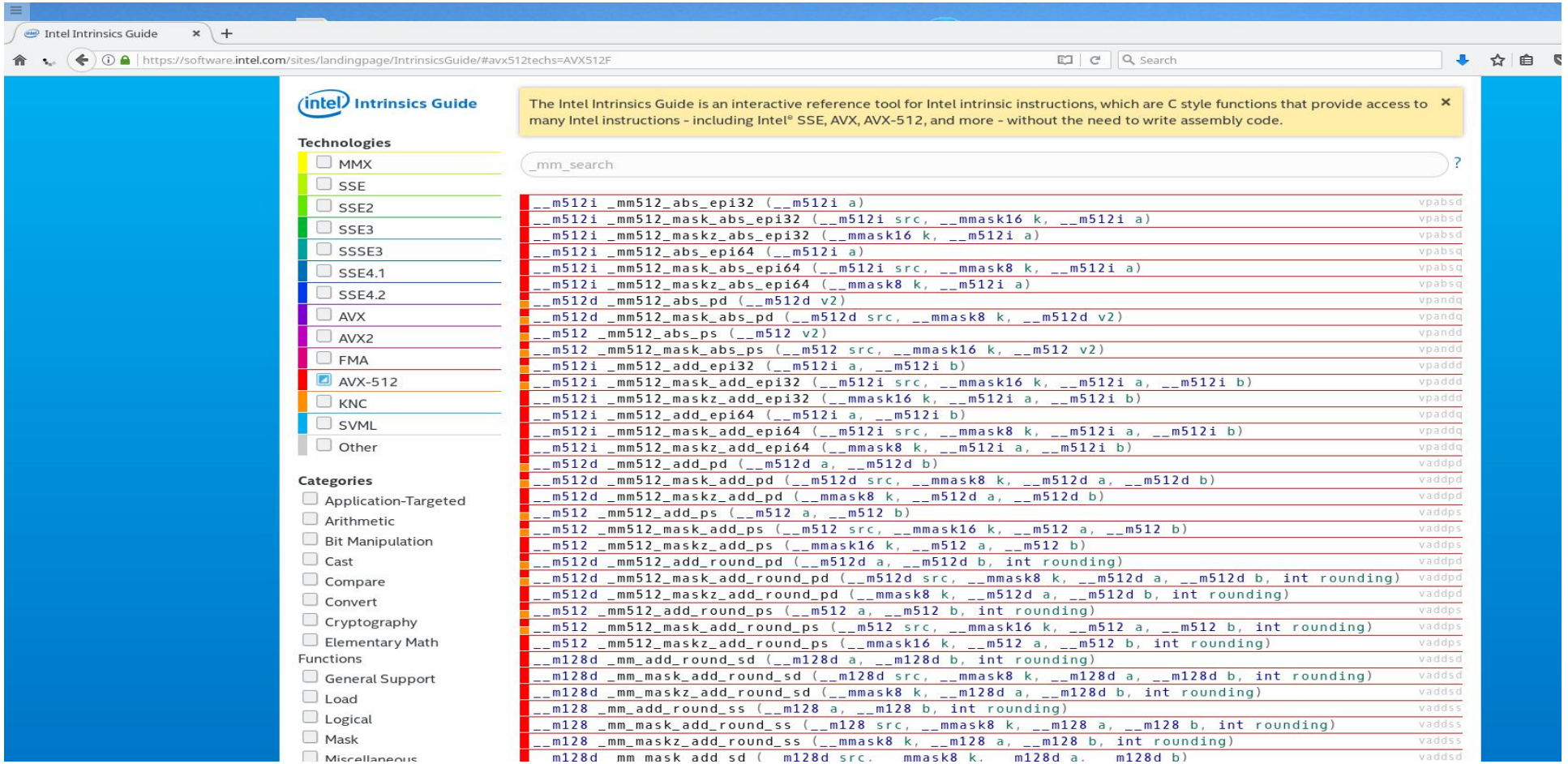

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- together with Intel`s AVX intrinsic guide (https://software.intel.com/sites/landingpage/IntrinsicsGuide)

=> this allowed us to start with the development of the AVX-512 kernels before the hardware was available

=> this lead to ~4000 lines of AVX-512 intrinsics code

Porting the kernels to AVX-512 - I

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- **Depending on the setup, 30% to 75% of runtime is spend in the back-transformation kernels**

Example code:

```
_mm512d h1, h2, q1, x1, y1, q2, x2, y2;

for(i = 2; i < nb; i++)
{
        h1 = _mm512_set1_pd(hh[i-1]);
        h2 = _mm512_set1_pd(hh[ldh+i]);

        q1 = _mm512_load_pd(&q[i*ldq]);
        x1 = _mm512_FMA_pd(q1, h1, x1);
        y1 = _mm512_FMA_pd(q1, h2, y1);
        q2 = _mm512_load_pd(&q[(i*ldq)+8]);
        x2 = _mm512_FMA_pd(q2, h1, x2);
        y2 = _mm512_FMA_pd(q2, h2, y2);
...
```

A problem turned out to be a compiler independent alignment of the data (and removing the effort from the users that build the ELPA library)

=> we had to use „posix_memalign“
For the data allocation and to ensure correct striding

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Porting the kernels to AVX-512 - II

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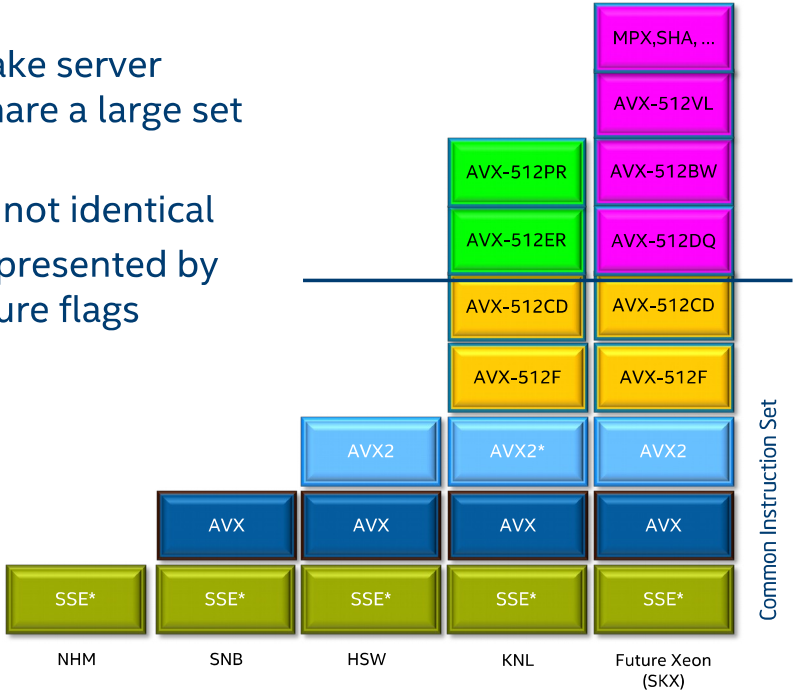
Programming AVX-512 intrinisics showed a little surprise:

On KNL some instructions are missing (compared to „old“ Xeons and upcoming SkyLake)

=> more code needed to program around
=> higher CPI

Reminder: AVX-512 – KNL and SKX

- KNL and SkyLake server architecture share a large set of instructions
  - but sets are not identical
- Subsets are represented by individual feature flags (CPUID)



Porting the kernels to AVX-512 - III

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Programming AVX-512 intrinisics showed a little surprise:

On KNL some instructions are missing (AVX-512DQ of normal xeon line)

=> more code needed to program around
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Reminder: AVX-512 – KNL and SKX

- KNL and SkyLake server architecture share a large set of instructions
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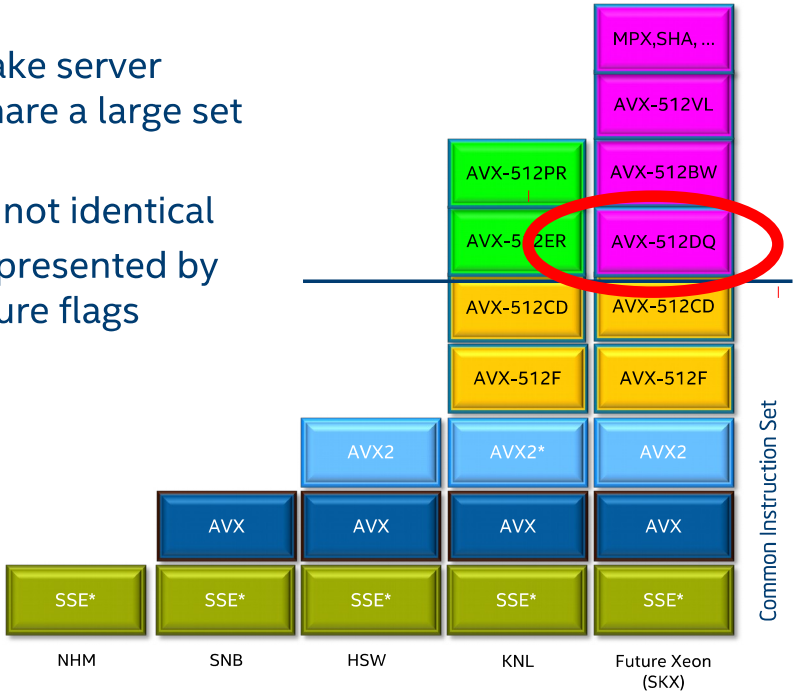
- Subsets are represented by individual feature flags (CPUID)



Porting the kernels to AVX-512 - IV

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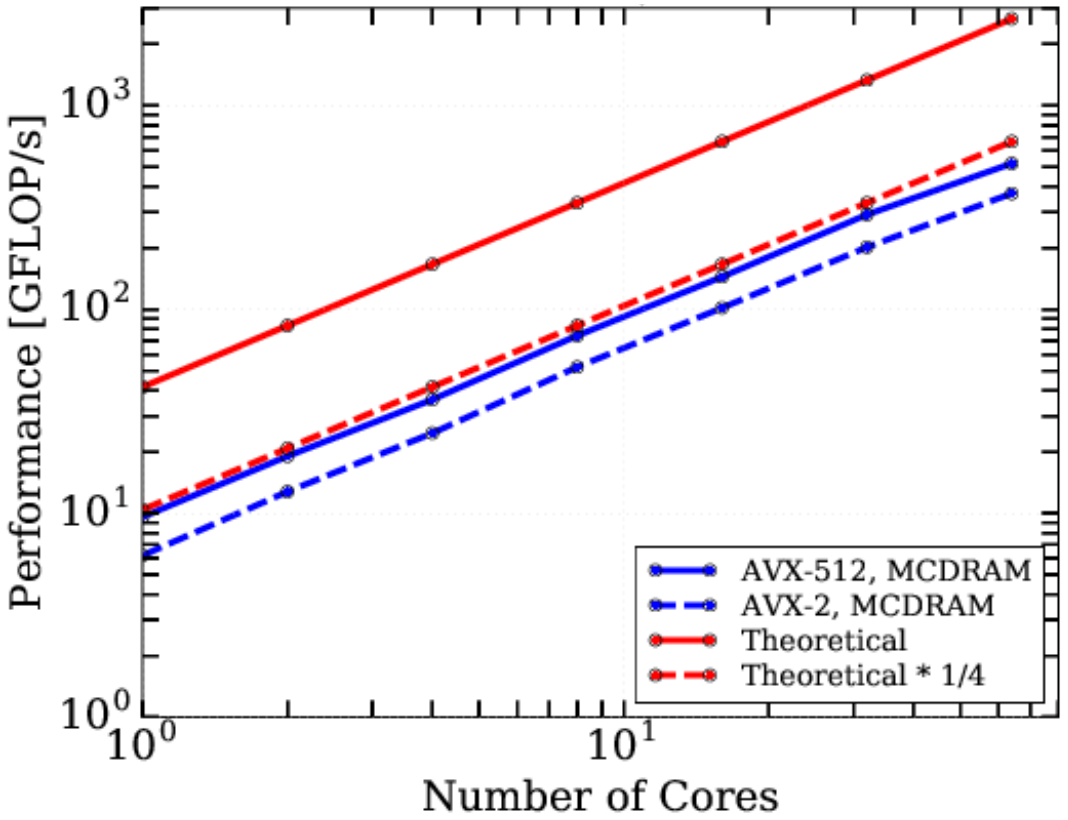

Theoretical limit:
1.3 GHz * 32 Flops/cycle * #cores
= 2.6 TFLOPS/s @ 64 cores

} Speedup AVX2 → AVX512 ~ 1.5x - 1.6x

double precision values!

ELPA @ 64 cores: ~520 GFLOPS/s

- ELPA measurments are ~ ¼ of theoretical value (ELPA is memory bound)
- we still work on improving this value; new version of Intel Advisor allows to measure the roofline directly (not yet done)

Porting the kernels to AVX-512 - V

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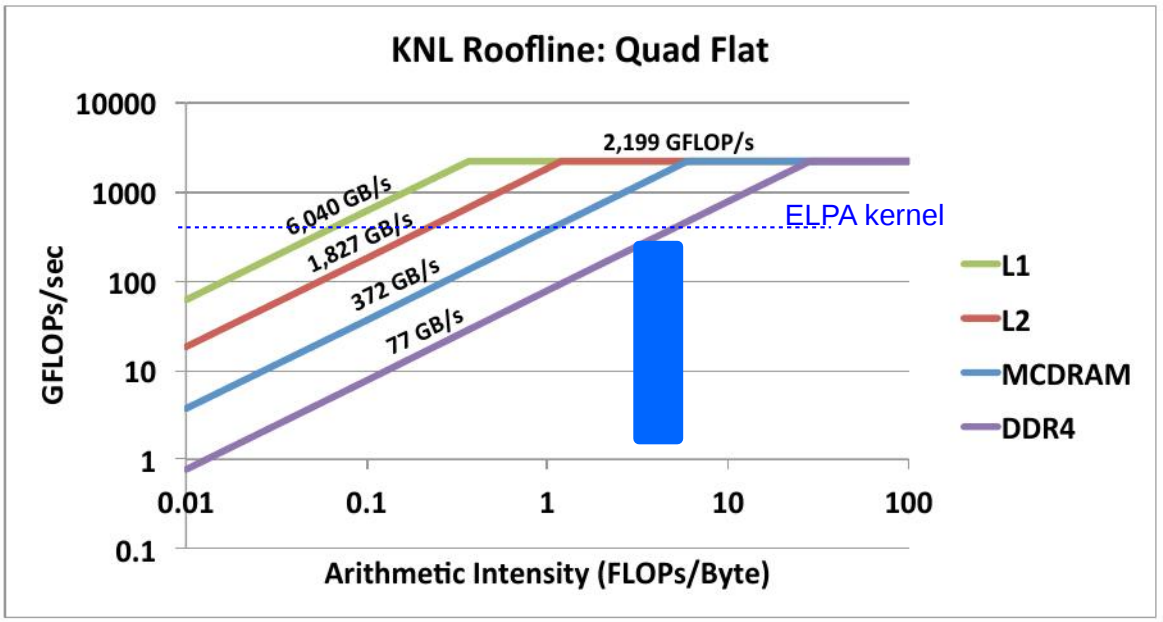

Theoretical limit:
1.3 GHz * 32 Flops/cycle * #cores
= 2.6 TFLOPS/s @ 64 cores

Speedup AVX2 → AVX512 ~ 1.5x-1.6x

memory bound
=> we can not expect peak

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Porting the kernels to AVX-512 - VI

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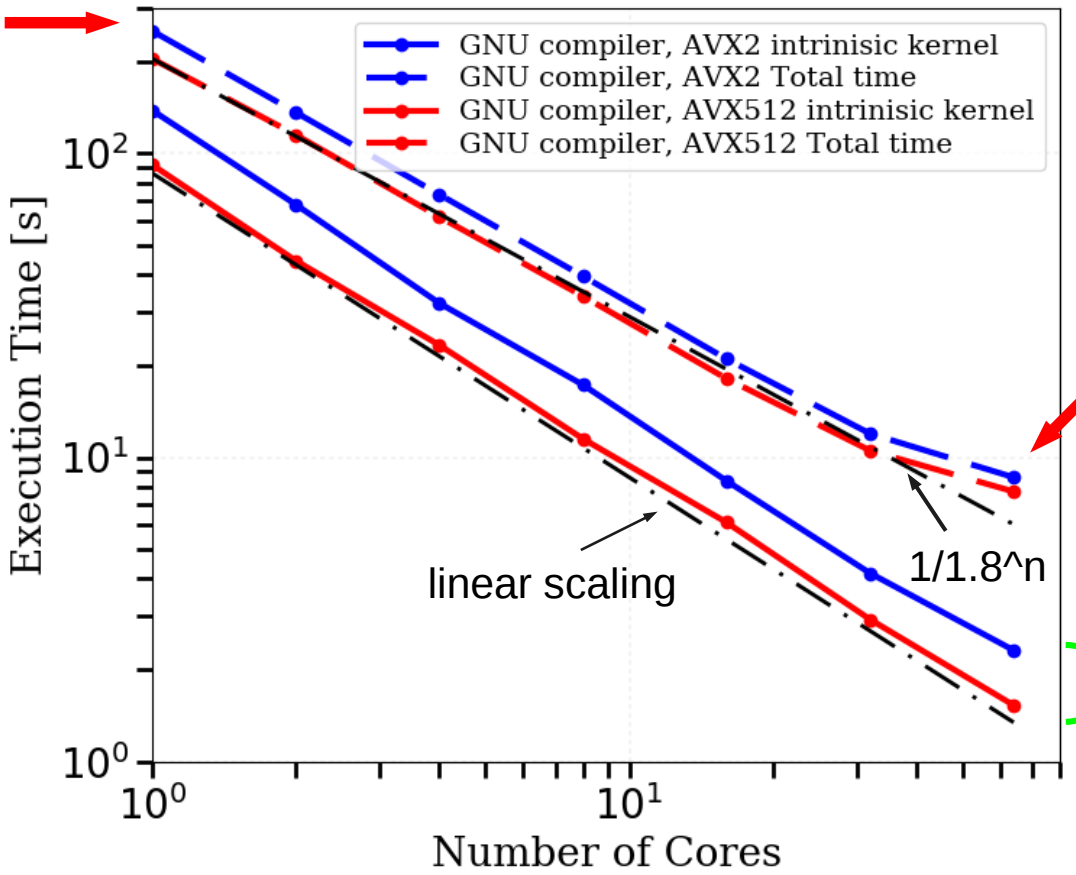
kernel ~ 44% of r.t.



kernel ~ 20% of r.t.

~ 1.3x

~ 1.5x - 1.6x for kernels
AVX2 → AVX512

Going to many nodes...

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- In a collaboration between the ELPA-AEO and the ELSI project (http://wordpress.elsi-interchange.org) it was possible to do first test of the ELPA library on the KNL system „THETA“ of the Argonne National Lab

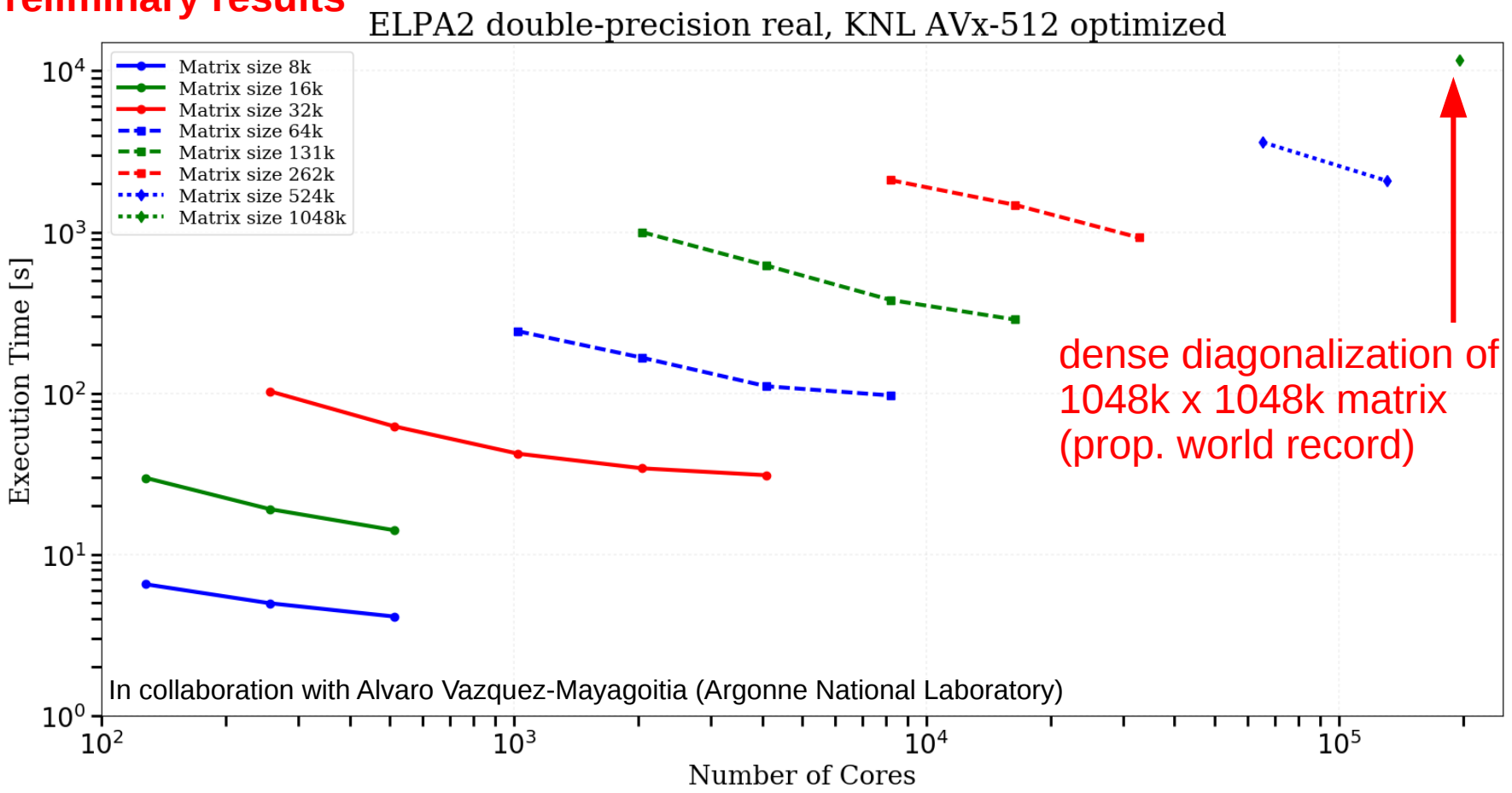
- All benchmarks have been performed by Vazquez-Mayagoit Alvaro (Argonne National Lab)

  => successful runs on up to 200.000 cores and a matrix size >1.000.000 could be demonstrated

  => we are still trying to improve the scaling on KNL

Going to many nodes...

Preliminary results



This research used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02-06CH1135

KNL experiences - Summary I

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General look and feel:

- it was straightforward to compile and run ELPA on KNL; first results after a few minutes

- architecture and software feels like a good old friend

- some initial surprises:

  a) compiler performance: in some setups GNU (gfortran + gcc) 6.1.0 was faster (up to 20%) than Intel (17.0.098); We have not checked again with newer versions of Intel 2017 or Intel 2018 beta. Propably this is not the case anymore

  b) documentation: it was not easy to find details like latency of MCDRAM (~190 ns), DRAM (~120 ns), …

  c) missing instructions on AVX-512 intrinsics

KNL experiences – Summary II

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Tools:

- **Intel SDE: fantastic tool, enabled writing and testing of AVX-512 kernels, before having access to real hardware**

- **Intel Advisor: very useful tool (and has improved a lot recently). Latest abillity to create roofline plots helps extremly (we could only use that up to now on Haswell systems)**

- **Intel Vtune: is a also very useful with interesting metrics (on Xeon processors) We found the advanced metrics on KNL less useful**

- **we percieve an „information gap“ between Vtune (high-level code analysis, low-level hardware information) and Advisor (detailed code analysis, most relevant metrics for advanced performance tuning):**

KNL experiences – Summary III

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It would have been helpful if we could have easily obtainded the following Information:

- **how much percentage of code is vectorized (total + subroutine level)**
- **what is the performance in GFlop/s (total + subroutine level)**
- **finding the arithmetic intensity (total + subroutine level)**
- **memory bandwidths used and data amount transferred (total + subroutine level)**
- **which parts of the code are memory bound or compute bound on KNL**

KNL experiences – Summary III

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- **memory bandwidths used and data amount transferred (total + subroutine level)**
- **which parts of the code are memory bound or compute bound on KNL**

Good perspective: with the new version of Intel Advisor (which we sadly do not yet have on our KNL system) a lot of these points are adressed!

=> In the near future we will be able to answer these questions for ELPA on KNL systems

Conclusions

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- As always: roofline analysis extremly helpful for performance optimisations
- We have ported the ELPA library to run on KNL clusters
- Writting AVX-512 intrinsic kernels proved to be necessary
- Successfull runs on up to ~200.000 cores have been demonstrated
- We are still working on improving the performance
  - detailed roofline analysis with new Advisor
  - cache blocking
  - but also trying libxsmm (dgemm sizes get small in ELPA during iteration)
- Some of the Intel tools (SDE, Advisor) were really helpfull for working on KNL
- The work on KNL is not yet finished ...

Questions?

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Thank you for your attention