CUG2016

London, UK, May 8 - 12

On Enhancing 3D-FFT Performance in VASP

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Outline

Many-core Optimizations in VASP

- From MPI to MPI + (OpenMP) Threading
- Multi-threaded FFT: MKL, FFTW (LibSci)
- 3D-FFT in VASP

How to improve FFT computation in VASP?

- FFTLIB: C++ template library to intercept FFTW calls
  - ❑ Plan Reuse
  - ❑ Composed FFT computation
  - ❑ …
- Some performance numbers

Many-core Optimizations in VASP

Many-core Optimizations in VASP

VASP – Vienna Ab-initio Simulation Package

- Electronic structure code
- MPI-only (latest official release)
- Implements DFT: many FFT computations

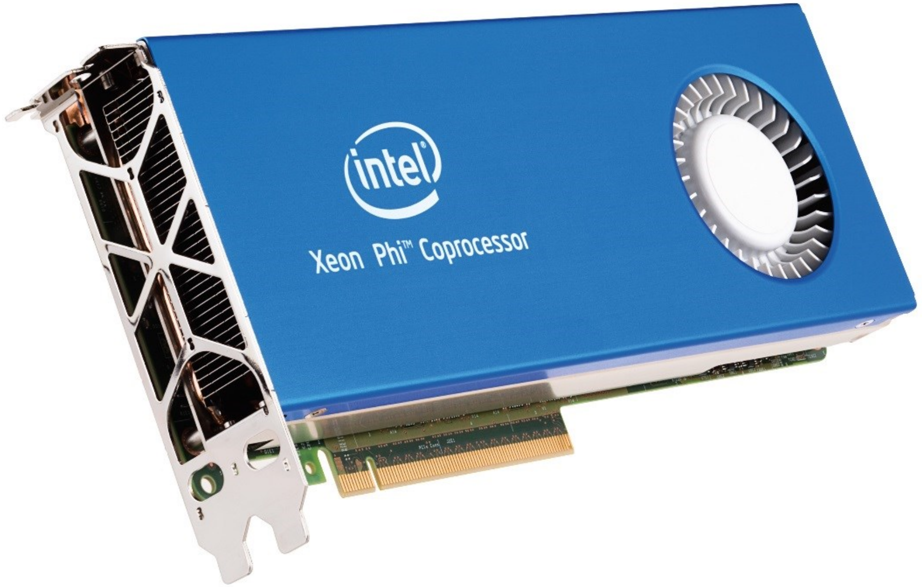
Optimization approach

- Introduce Threading
- Optimize code sections for SIMD (talk at CUG2015)
- Improve library integration/usage: FFT, BLAS/Scalapack, …

Many-core Optimizations in VASP

Many-core processor = lots of (lightweigth) compute cores on a chip

- Intel Xeon Phi KNC/KNL: 60+ cores
- Highly parallel computation
- MPI-only will not work in the majority of cases



MPI + (OpenMP) Threading

- KNL: 4, 8, 16 MPI ranks + lots of (OpenMP) threads
- User function part: code instrumentation via OpenMP compiler directives
- Library functions: multi-threaded context or call to multi-threaded library

Many-core Optimizations in VASP

Current state of VASP* optimization

- MPI + OpenMP: almost fully adapted code base
- SIMD: OpenMP 4.x directives
- Multi-threaded FFT computation
  - 3D-FFT where possible: it is really fast!
  - “Ball ↔ Cube” FFT optimization: composed 1D+1D+1D FFT

*This VASP version is not yet officially available! Will be coming soon ☺

Many-core Optimizations in VASP

3D-FFT in VASP

- FFTW library calls: Intel MKL can be used through its FFTW interface
- Calling scheme in VASP:

```
// create plan
p=fftw_plan_xxx(…)

// execute
fftw_execute(p)

// destroy plan
fftw_destroy_plan(p)
```

This happens again and again

Many-core Optimizations in VASP

3D-FFT in VASP

- Program performance (PdO2: Paladiumdioxid on Paladium surface)

  24 MPI ranks on 4 Cray XC-40 compute nodes (Haswell), T=1,4 threads per rank
  MKL 11.3.2, FFTW (from GitHub and Cray LibSci)

	Setup: PdO2					
	MKL 11.3.2		FFTW		FFTW (LibSci)	
	T=1	T=4	T=1	T=4	T=1	T=4
Total	146.6s	78.0s	162.1s	122.5s	162.3s	121.9s
3D-FFT	23.4s	10.7s	38.2s	43.3s	38.6s	41.9s
+planner	1.0s	1.0s	10.0s	32.9s	9.8s	31.1s
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A lot of time is spent in the planner phase!

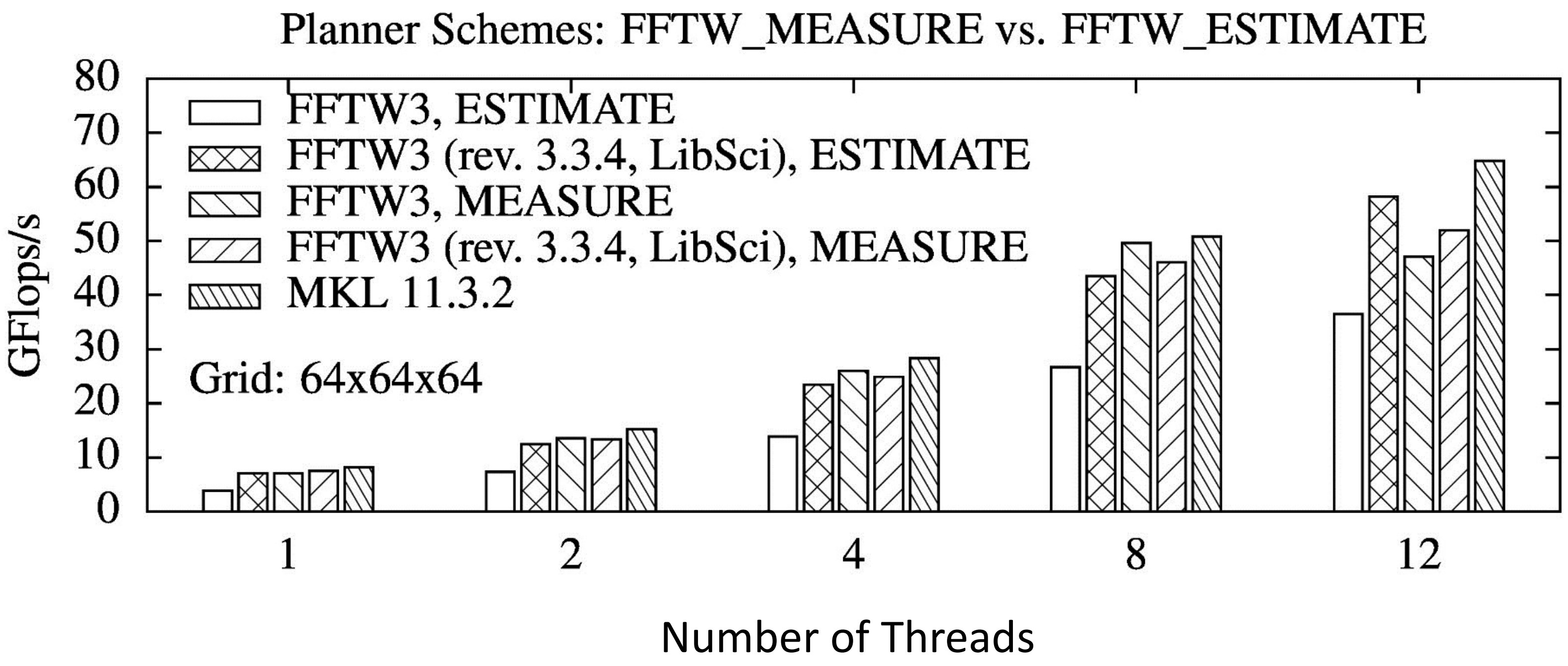
Many-core Optimizations in VASP

3D-FFT in VASP

- FFTW provides different planner schemes: ESTIMATE, MEASURE, …

  ESTIMATE – cheap

  MEASURE – expensive: kind of online-autotuning on different FFT algorithms



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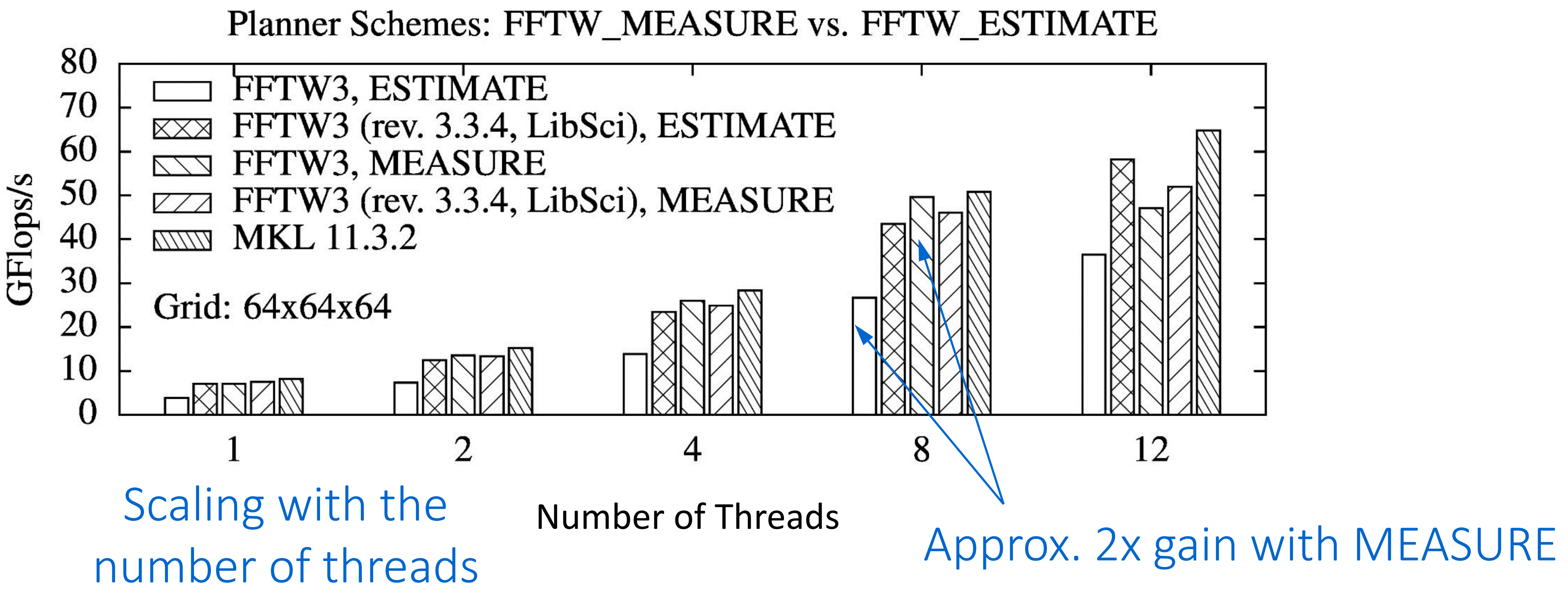
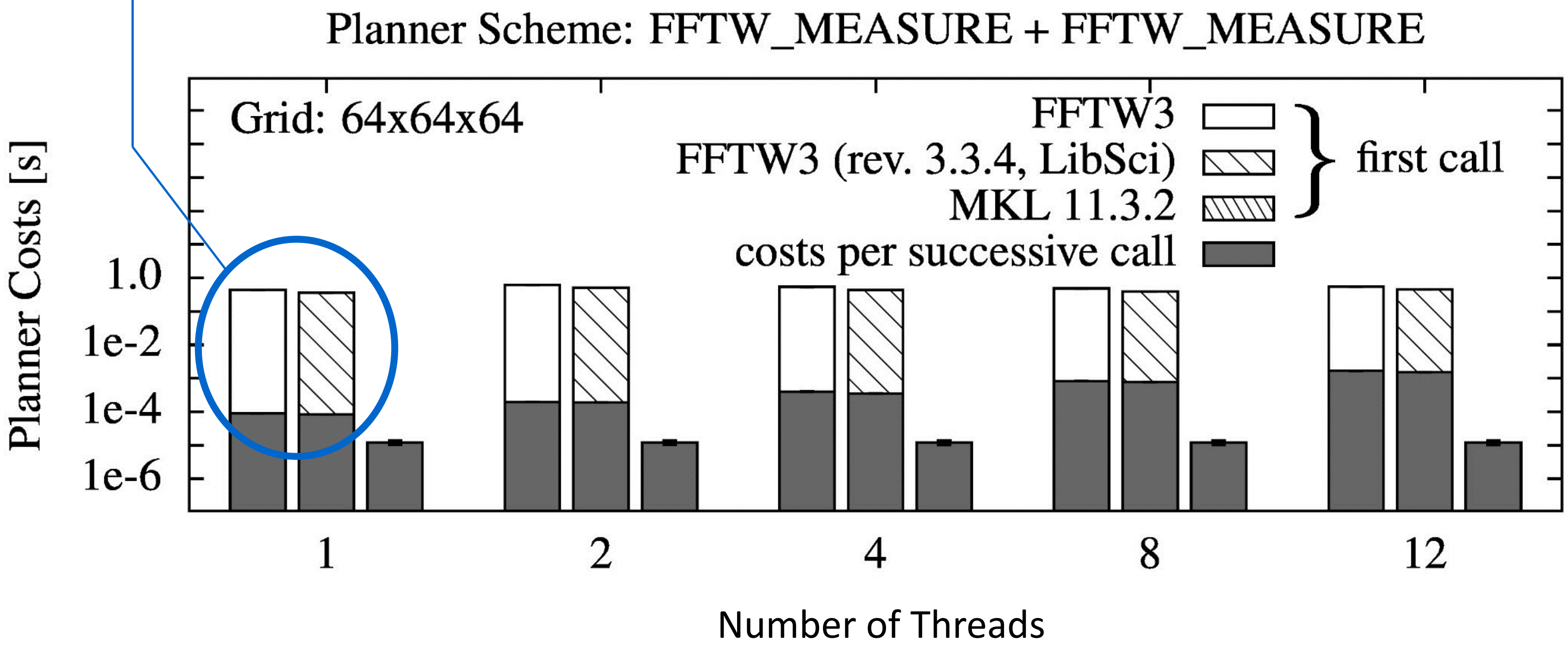


Many-core Optimizations in VASP

3D-FFT in VASP

- Costs for planning with MEASURE and using the FFTW Wisdom feature for faster plan creation



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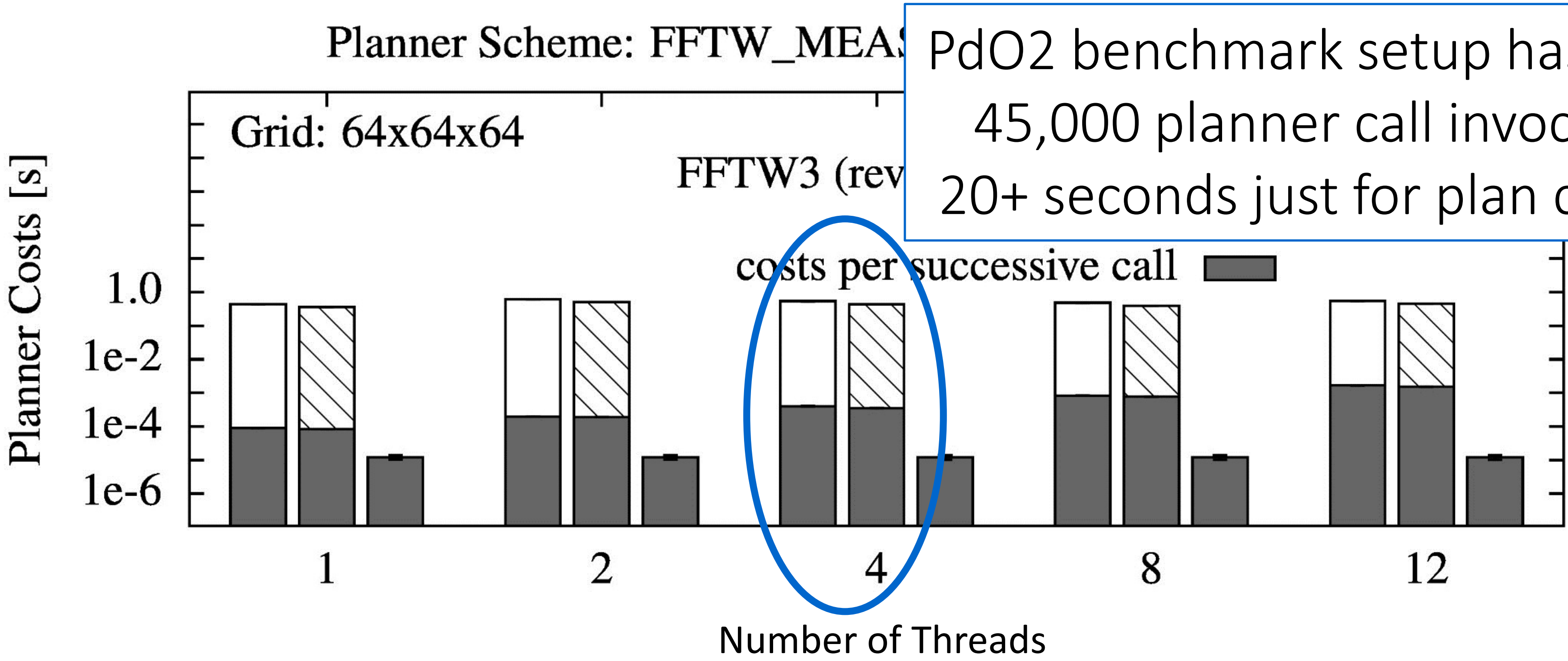

PdO2 benchmark setup has approx. 45,000 planner call invocations: 20+ seconds just for plan creation!

Many-core Optimizations in VASP

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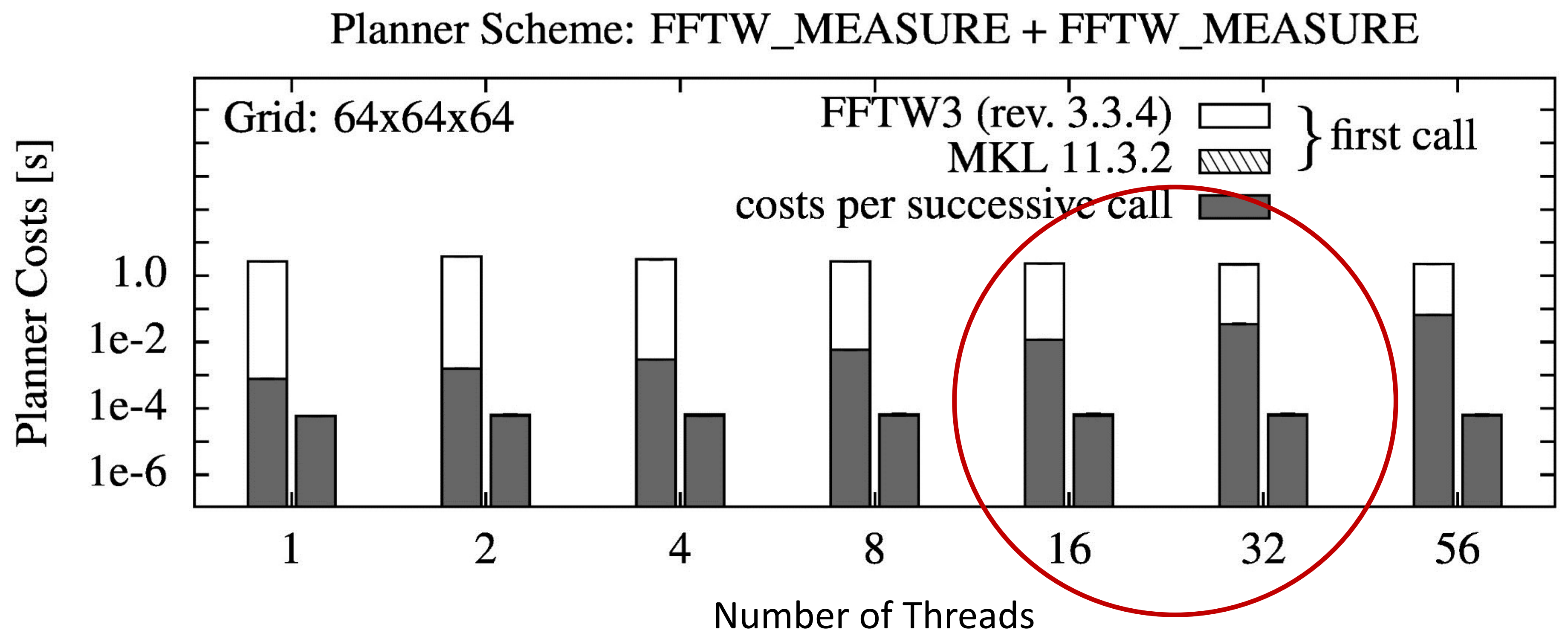
Xeon Phi (KNC) Data



Many-core Optimizations in VASP

3D-FFT in VASP

- Costs for plan creation seems to become dominant with increasing number of threads to be used for the computation

Can we do better?

How to Improve FFT Computation in VASP?

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Main issue when using FFTW: plan creation

- Recommendation on FFTW webpage: “reuse plans as long as possible”
- Plan caching mechanism in the application?
  No, create a library for that purpose!

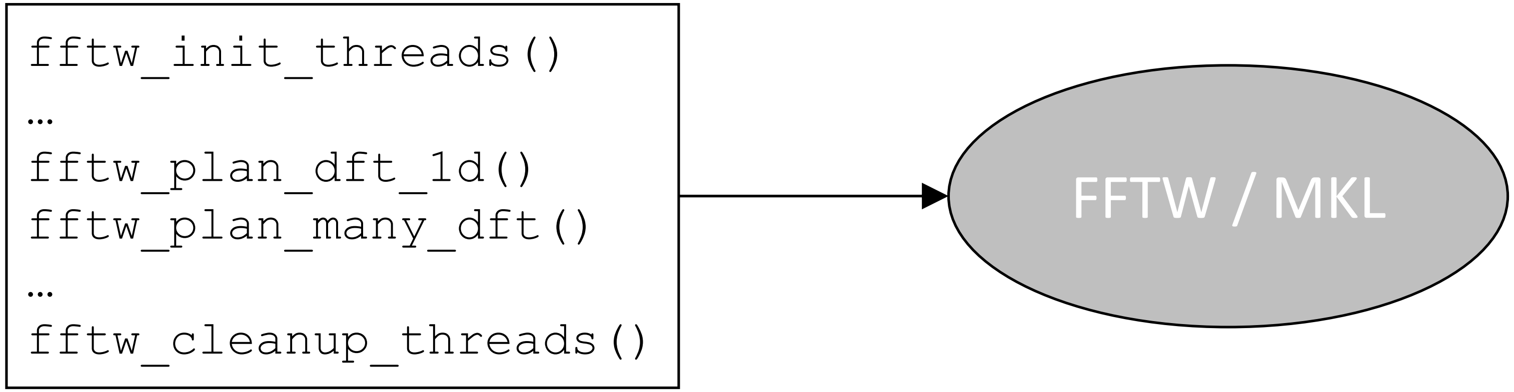
FFTLIB (will be hosted as open source library soon)

- C++ template library encapsulation FFTW and DFTI specifics
- Plan reuse: hash-map + cache
- Composed FFT
  - “Ball ↔ Cube” FFT optimization
  - Skip transpose operation(s)
  - High Bandwidth Memory (preparation for Intel’s Xeon Phi KNL)

How to Improve FFT Computation in VASP?

FFTLIB – Approach

- Intercept FFTW calls + additional features



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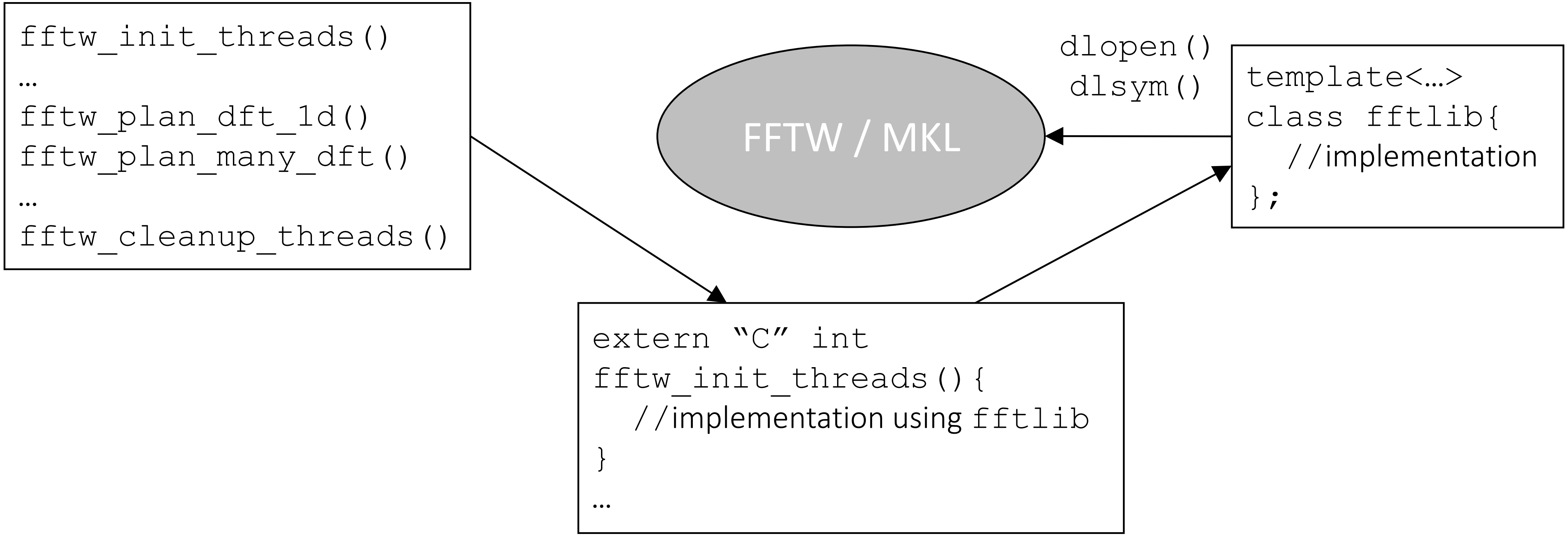
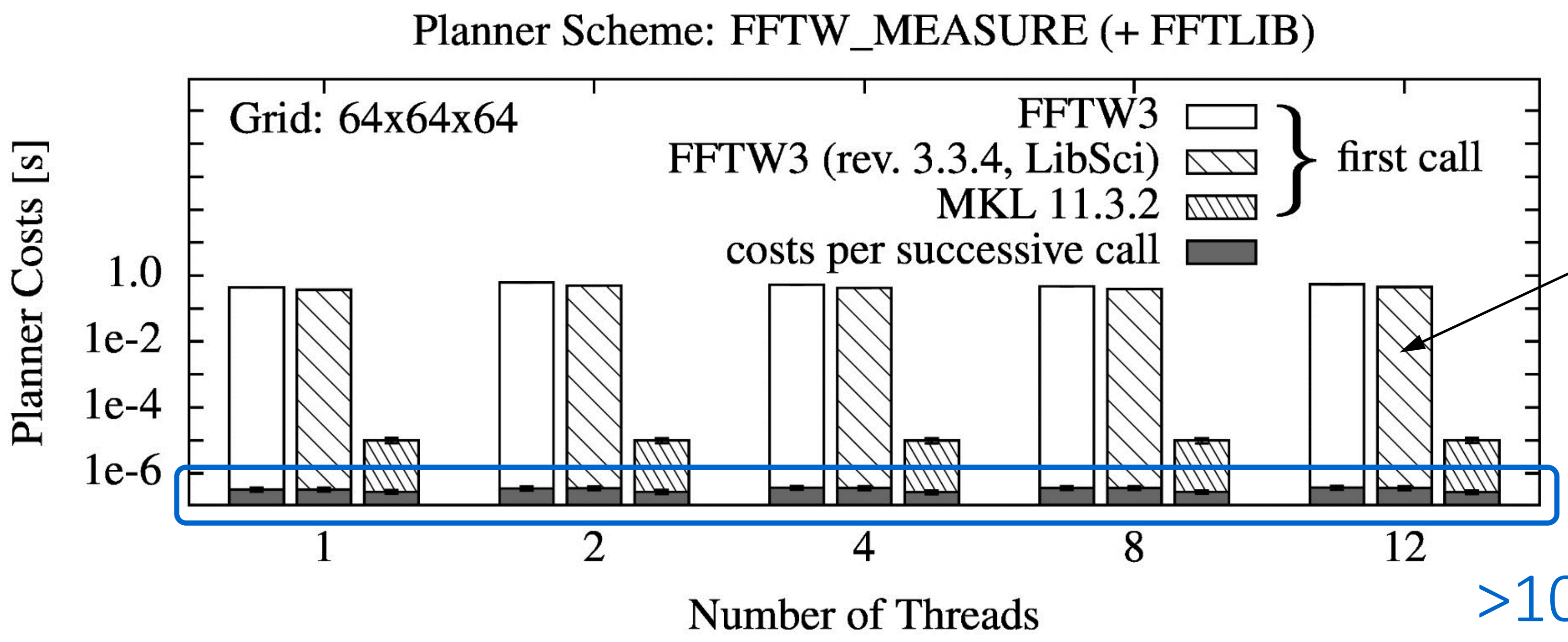


How to Improve FFT Computation in VASP?

FFTLIB – Plan Reuse

- Plans are stored permanently in a hash-map + cache
  - ❑ First planner call goes to FFTW / MKL for each geometry
  - ❑ Successive planner calls are served by FFTLIB



Remains the same

0.3μs – 0.4μs request time: >1000x gain for FFTW

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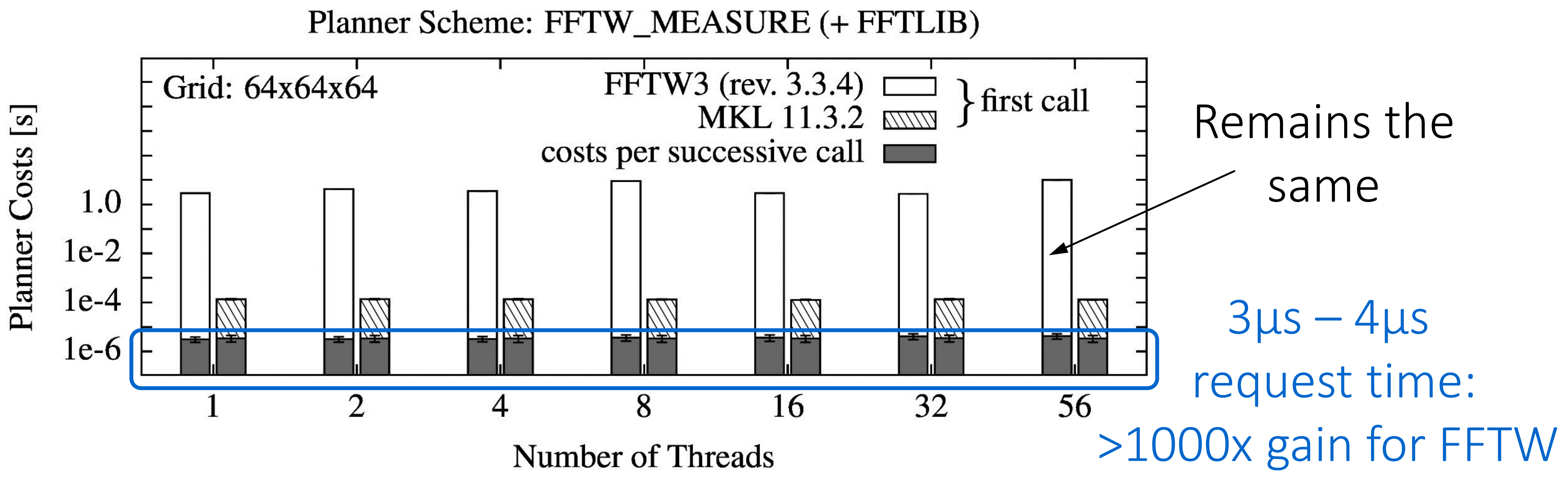

How to Improve FFT Computation in VASP?

3D-FFT in VASP with FFTLIB

- Program performance (PdO2: Paladiumdioxid on Paladium surface)

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	T=1	T=4	T=1	T=4	T=1	T=4
Total	145.5s	84.8s	152.6s	86.5s	153.3s	90.0s
3D-FFT	23.4s	10.0s	29.0s	11.3s	29.6s	11.7s
+ planner	0.3s	0.3s	0.8s	0.9s	0.8s	0.9s
+ execute	22.4s	9.7s	28.2s	10.4s	28.8s	10.8s

Without FFTLIB:
Approx. 32 seconds (T=4) just for plan creation with FFTW

Only the initial planner costs contribute

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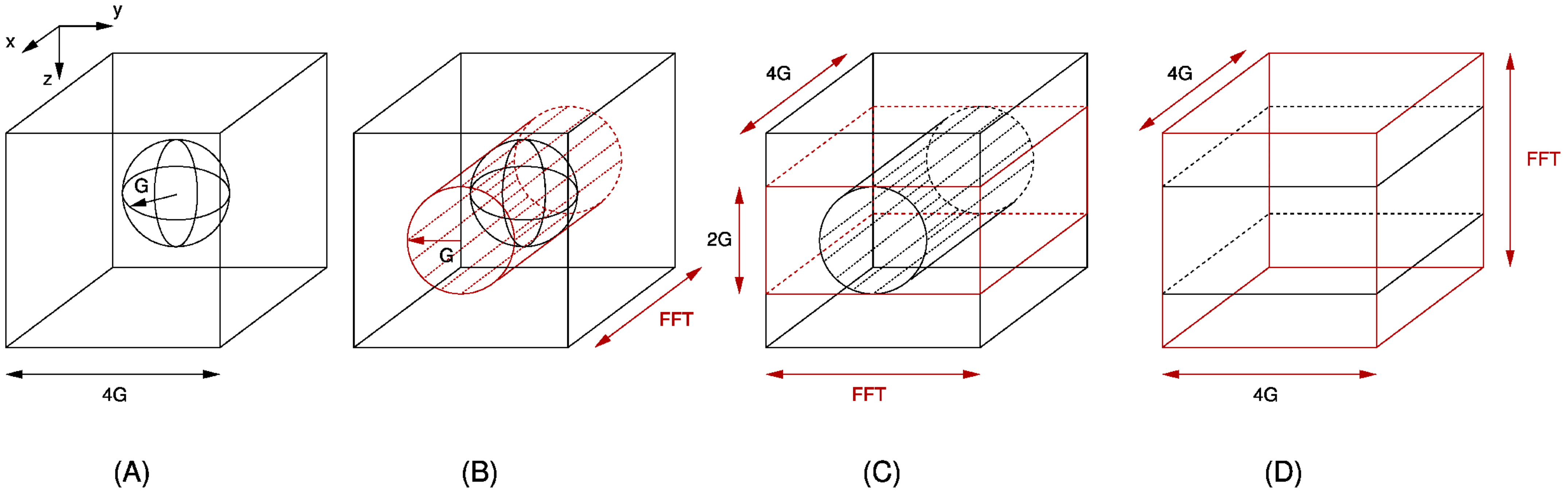
How to Improve FFT Computation in VASP?

3D-FFT with FFTLIB

- Composed FFT: "Ball ↔ Cube" FFT optimization (optional)
  - Reciprocal space vector *G* below a certain cutoff

This is what VASP is doing right now



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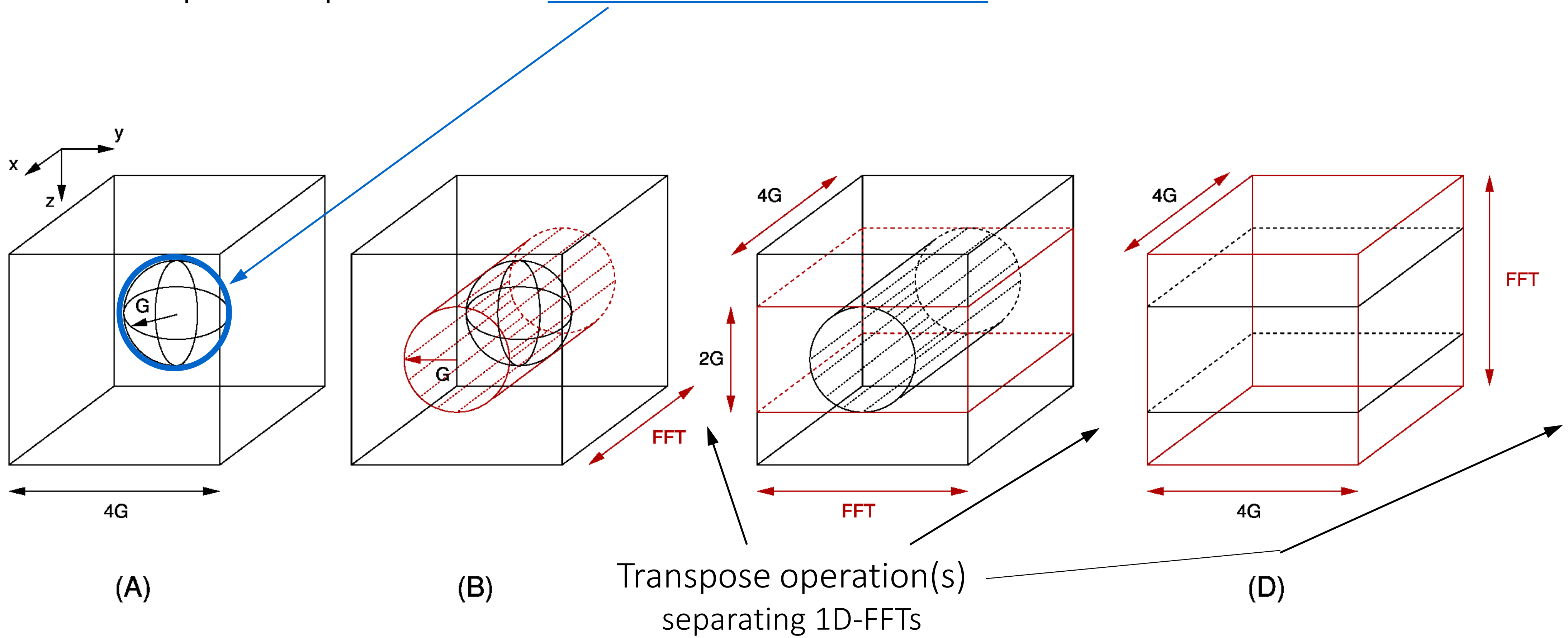

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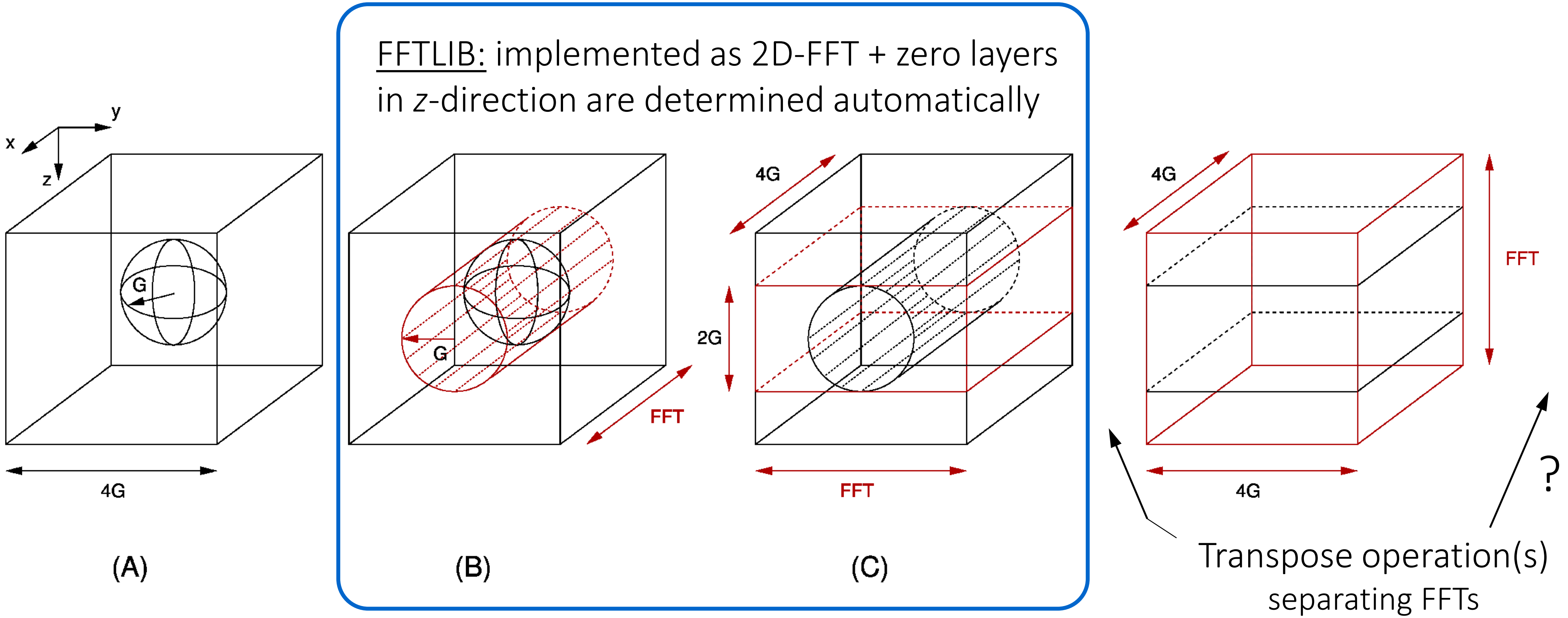
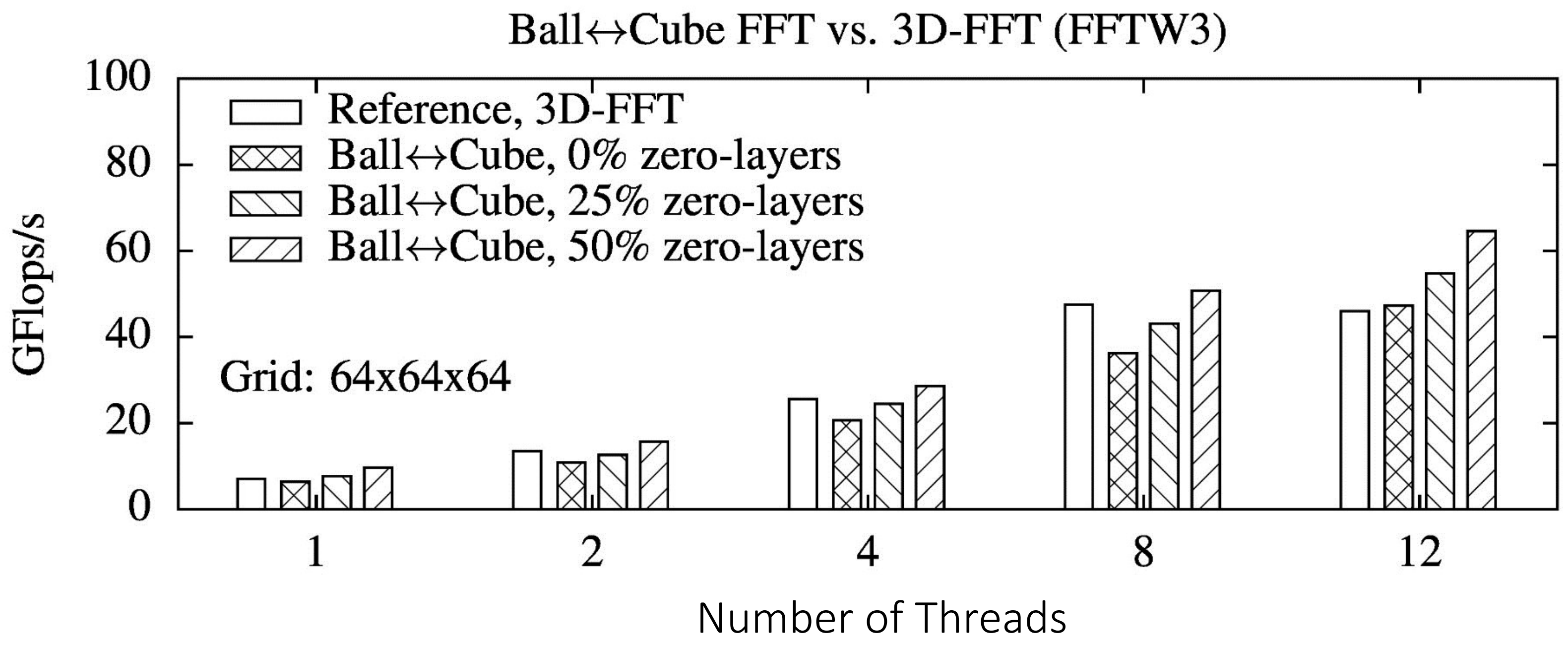


How to Improve FFT Computation in VASP?

3D-FFT with FFTLIB

- Composed FFT: “Ball ↔ Cube” FFT optimization + skip last transpose
  - ❑ Synthetic benchmark kernel: here for FFTW, but similar for MKL
  - ❑ Not yet integrated into VASP



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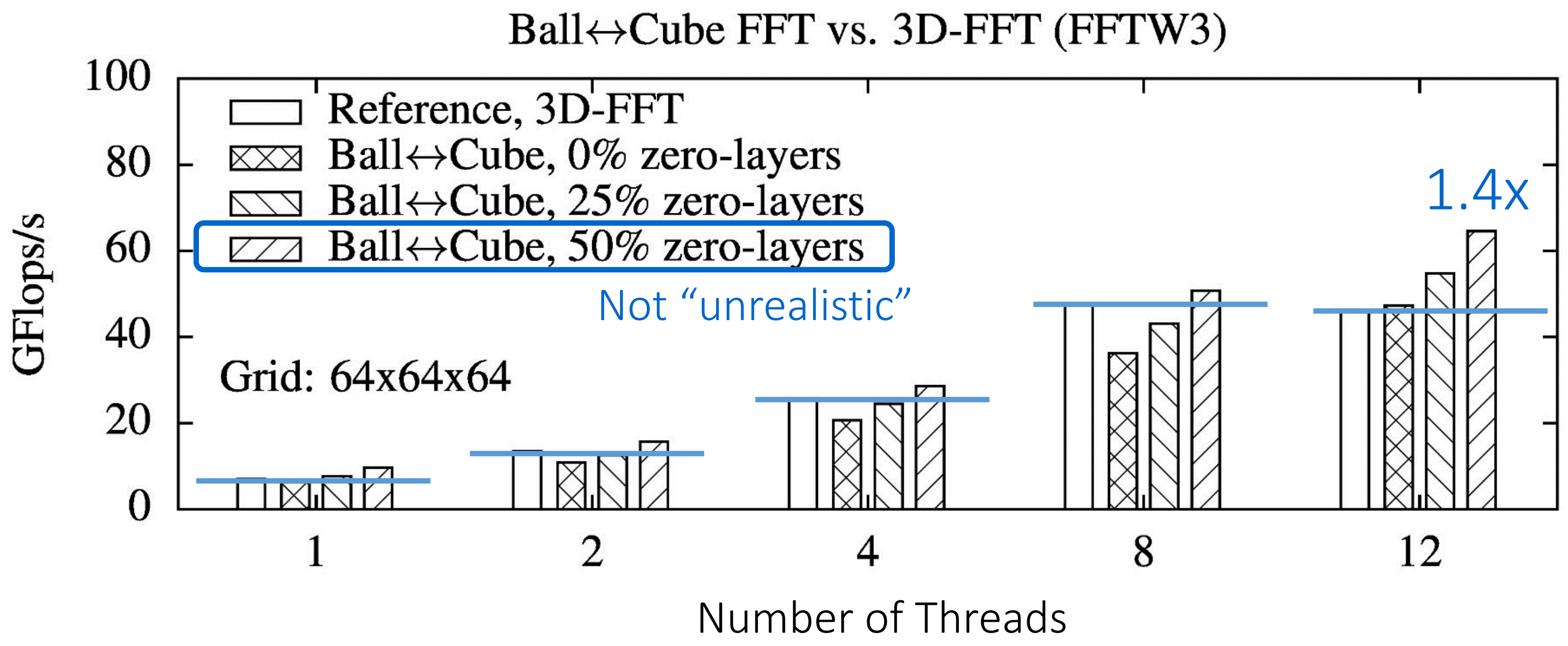

Summary

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Many-core optimization in VASP

- MPI + OpenMP, SIMD
- Multi-threaded library calls: 3D-FFT in this talk
  - ❑ Scaling quite acceptable
  - ❑ Issue with plan creation when using FFTW: consumes a lot of time

FFTLIB: C++ template library intercepting FFTW calls

- Plan reuse via hash-map + cache: up to 1.4x for VASP application with FFTW
- Composed 3D-FFT: 1.4x with FFTW when skipping last transpose

Not shown here (but in the paper)

- High bandwidth memory usage (memkind): 10% gain for transpose
- Autotuning within FFTLIB: just an outlook

Acknowledgement

Jeongnim Kim (Intel, US)

Funding:

Research Center for Many-core HPC (IPCC@ZIB)

Partners:

ZIB + VASP developer team (Georg Kresse, Martijn Marsman)

Joint research project ZIB + Cray