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 (lightweight) 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:

```c
// 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)

<table>
<thead>
<tr>
<th>24 MPI ranks on 4 Cray XC-40 compute nodes (Haswell), T=1,4 threads per rank</th>
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<td>78.0s</td>
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**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)**
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, FTWF (from GitHub and Cray LibSci)

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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

![Graph showing planner schemes for FFTW: FFTW3, FFTW3 (rev. 3.3.4, LibSci), FFTW3, MKL 11.3.2]
Many-core Optimizations in VASP

3D-FFT in VASP

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```
FFT3, ESTIMATE
FFT3 (rev. 3.3.4, LibSci), ESTIMATE
FFT3, MEASURE
FFT3 (rev. 3.3.4, LibSci), MEASURE
MKL 11.3.2
```

Grid: 64x64x64

Scaling with the number of threads

Approx. 2x gain with MEASURE
Many-core Optimizations in VASP

3D-FFT in VASP

- Costs for planning with MEASURE and using the FFTW Wisdom feature for faster plan creation
Many-core Optimizations in VASP

3D-FFT in VASP

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

PdO2 benchmark setup has approx. 45,000 planner call invocations: 20+ seconds just for plan creation!
Many-core Optimizations in VASP

3D-FFT in VASP

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

Planner Scheme: FFTW_MEASURE + FFTW_MEASURE

Grid: 64x64x64

Number of Threads:
- 1
- 2
- 4
- 8
- 16
- 32
- 56

Planner Costs [s]

- 1.0
- 1e-2
- 1e-4
- 1e-6

FFT3W (rev. 3.3.4)
MKL 11.3.2

} first call

costs per successive call

wende@zib.de  On Enhancing 3D-FFT Performance in VASP  CUG2016, London, UK
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?
How to Improve FFT Computation in VASP?

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

```
fftw_init_threads()
...
fftw_plan_dft_1d()
fftw_plan_many_dft()
...
fftw_cleanup_threads()
```
How to Improve FFT Computation in VASP?

FFTLIB – Approach

- Intercept FFTW calls + additional features

```c
extern "C" int
fftw_init_threads(){
    //implementation using fftlib
}
```

```cpp
template<...>
class fftlib{
    //implementation
};
```
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

Planner Scheme: FFTW_MEASURE (+ FFTLIB)

Remains the same

0.3µs – 0.4µs request time:

>1000x gain for FFTW
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
3µs – 4µs request time:
>1000x gain for FFTW

Xeon Phi (KNC) Data
How to Improve FFT Computation in VASP?

3D-FFT in VASP with FFTLIB

- 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)

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<td>T=1</td>
<td>T=4</td>
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<tr>
<td>Total</td>
<td>145.5s</td>
<td>84.8s</td>
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Without FFTLIB: Approx. 32 seconds (T=4) just for plan creation with FFTW

Only the initial planner costs contribute
How to Improve FFT Computation in VASP?

3D-FFT in VASP with FFTLIB

- Program performance (PdO2: Palladium dioxide on Palladium surface)
  24 MPI ranks on 4 Cray XC-40 compute nodes (Haswell), T=1,4 threads per rank
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<td>1.01x</td>
<td>0.92x</td>
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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
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

(A) \( 4G \)

(B) \( 2G \)

Transposition operation(s) separating 1D-FFTs

(D) \( 4G \)
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

FFTLIB: implemented as 2D-FFT + zero layers in $z$-direction are determined automatically

(x, y, z)
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

![Graph comparing Ball↔Cube FFT and 3D-FFT performance](image)

- Grid: 64x64x64
- Number of Threads: 1, 2, 4, 8, 12
- GFlops/s: 0 to 100
- Reference, 3D-FFT
- Ball↔Cube, 0% zero-layers
- Ball↔Cube, 25% zero-layers
- Ball↔Cube, 50% zero-layers

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On Enhancing 3D-FFT Performance in VASP

CUG2016, London, UK
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

![Graph showing comparison between Ball↔Cube FFT and 3D-FFT (FFTW3)]

- Grid: 64x64x64
- Number of Threads: 1, 2, 4, 8, 12
- GFlops/s
- Reference, 3D-FFT
- Ball↔Cube, 0% zero-layers
- Ball↔Cube, 25% zero-layers
- Ball↔Cube, 50% zero-layers

Not “unrealistic”
Summary
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

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