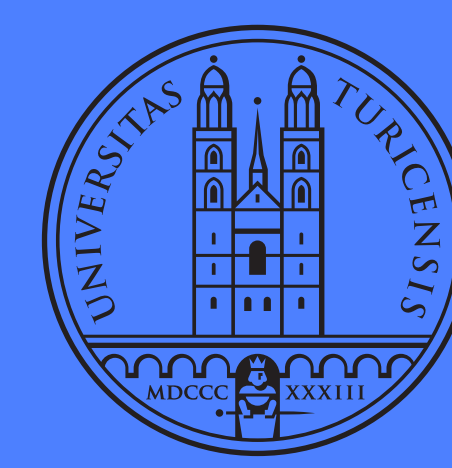




WANNIER BERRI: an advanced tool for interpolation of Berry curvature and related quantities. (aka Wannier19)

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Anomalous Hall and Nernst effects

The AHC tensor is given by:

$$\sigma_{\alpha\beta}^{\text{AHE}}(0) = -\frac{e^2}{\hbar} \int \frac{d\mathbf{k}}{(2\pi)^3} \sum_n f_{n\mathbf{k}} \Omega_{n,\alpha\beta}(\mathbf{k}) \quad (1)$$

in terms of Berry curvature:

$$\Omega_{n,\alpha\beta}(\mathbf{k}) = -2\text{Im} \langle \nabla_{k_\alpha} u_{n\mathbf{k}} | \nabla_{k_\beta} u_{n\mathbf{k}} \rangle. \quad (2)$$

where $|u_{n\mathbf{k}}\rangle = e^{-i\mathbf{k}\cdot\mathbf{r}}|\psi_{n\mathbf{k}}\rangle$ is the cell-periodic Bloch function. to evaluate it one needs:

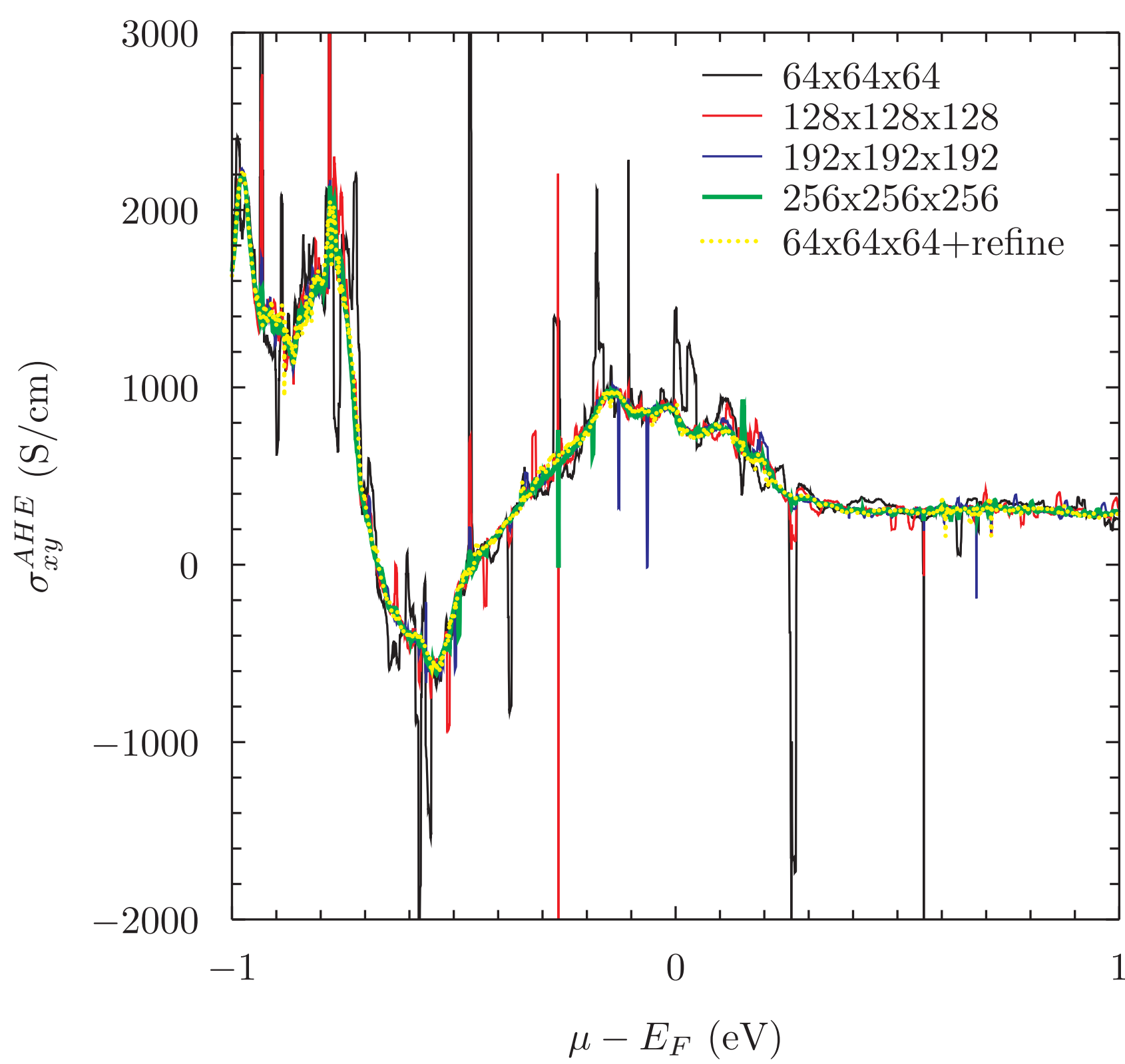
- ▶ a smooth gauge
- ▶ dense grid of \mathbf{k} -points

That is where Wannier interpolation helps a lot.

Anomalous Nernst Effect is even harder

$$\alpha_{xy}^{\text{ANE}} = -\frac{1}{e} \int d\varepsilon \frac{\partial f}{\partial \varepsilon} \sigma_{xy}^{\text{AHE}}(\varepsilon) \frac{\varepsilon - \mu}{T} \quad (3)$$

because at low T it is essentially the derivative of σ^{AHE}



Irudia 1: Example: AHC of bcc Fe as a function of chemical potential μ , for different interpolation grids, with and without recursive refinement

Overview

W-BERRI is an improved python implementation of postw90.x part of **Wannier90**.

W-BERRI accepts the Wannier functions generated by Wannier90, or any tight-binding model. Than a BZ integral of any combination of velocities, Berry curvatures and other k-space quantities can be evaluated.

postw90.x is **good**, because it

- ▶ is a well-established code
- ▶ known for ages
- ▶ has a broad community of developers
- ▶ has many implemented features
- ▶ (many more)

W-BERRI is **better**, because it

- ▶ is faster
- ▶ Employs a mixture of fast and slow Fourier transforms
- ▶ uses recursive adaptive refinement for accurate evaluation around special points in BZ
- ▶ accounts for the symmetries, to integrate only the irreducible part of BZ and make the result symmetric.
- ▶ is written in object-oriented Python, which allows easier further development.
- ▶ has some more efficient algorithms, in particular
 - ▶ for multiple Fermi levels
 - ▶ minimal-distance replica selection method

Hosted on github

<https://github.com/stepan-tsirkin/wannier-berri>

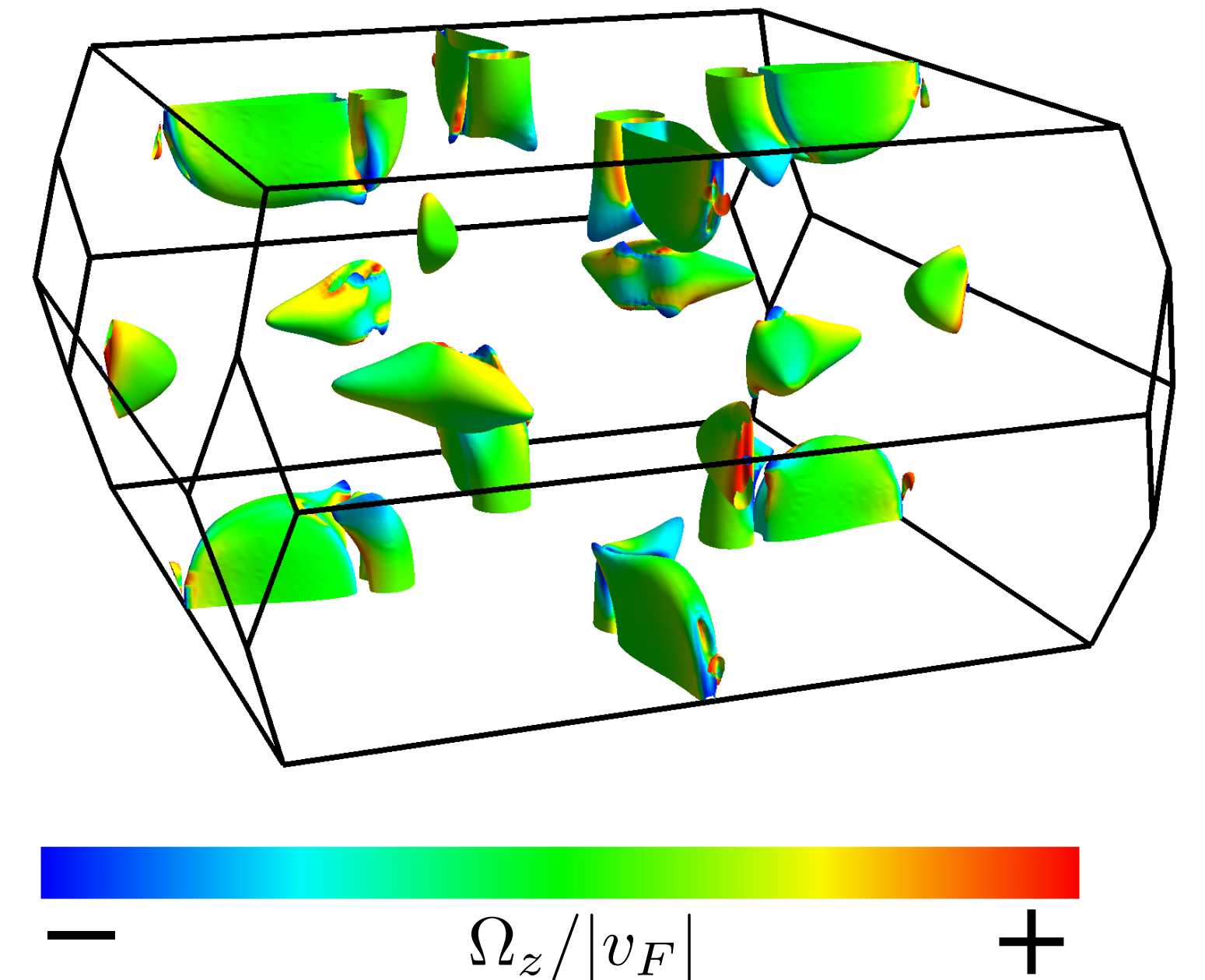


Install with pip

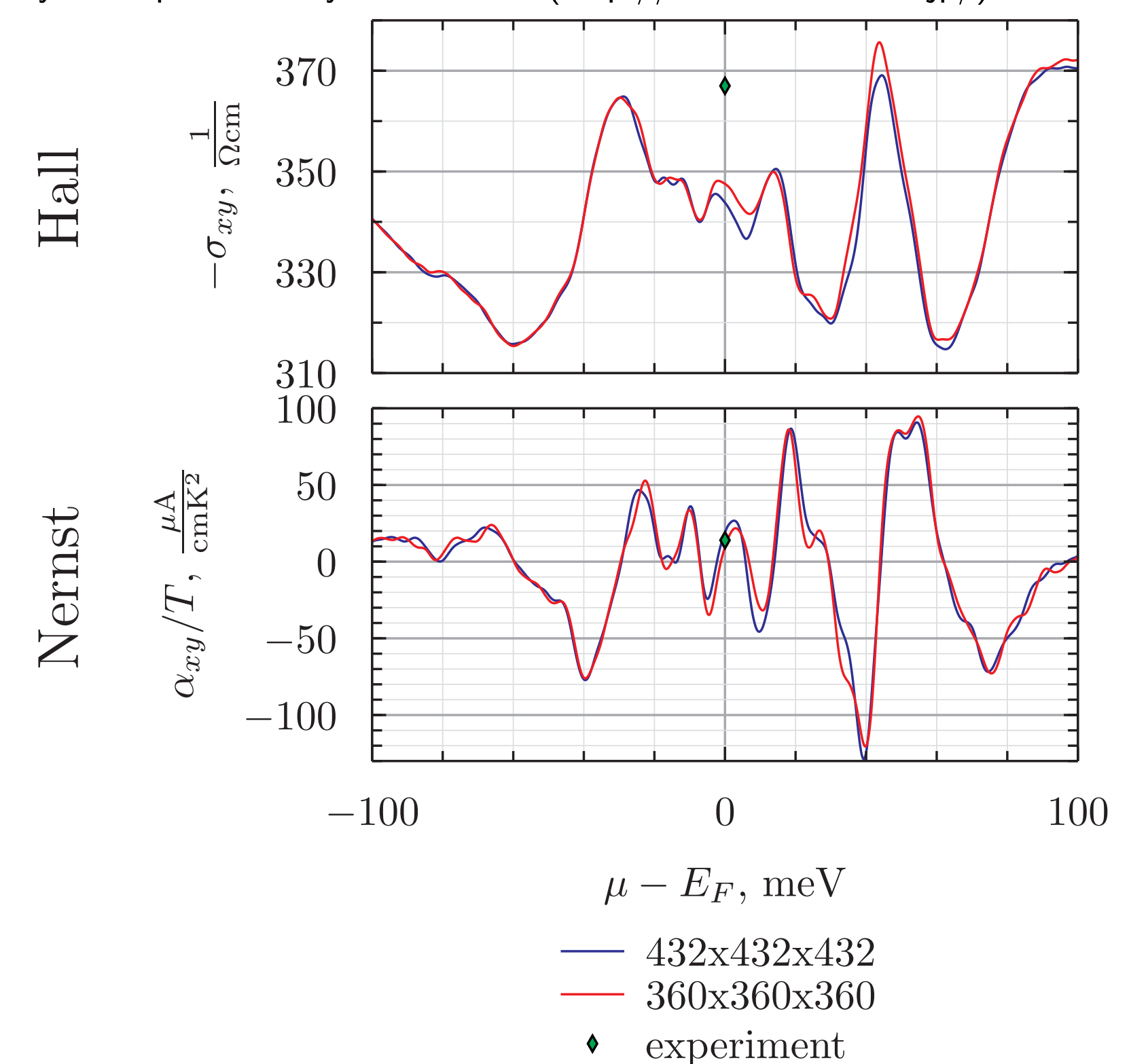
pip3 install wannierberri

First real-life use: AHE and ANE in magnetic Weyl Semimetal PrAlGe

"Magnetism and anomalous transport in the Weyl semimetal PrAlGe: possible route to axial gauge fields". D. Destraz, L. Das, S.S. Tsirkin, Y. Xu, *et al.* Accepted in **npj Quantum Materials**.



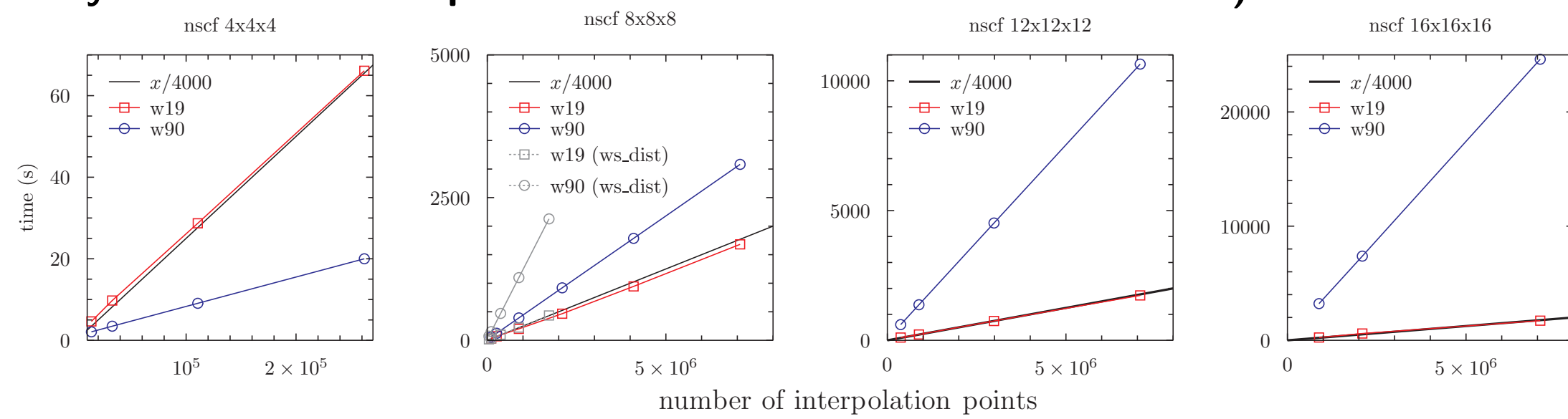
Irudia 2: Fermi surface of ReAlGe coloured by Berry curvature divided by Fermi velocity. Plot produced by FermiSurfer (<http://fermisurfer.osdn.jp/>)



Irudia 3: AHE and ANE calculated in PrAlGe in comparison with experiment

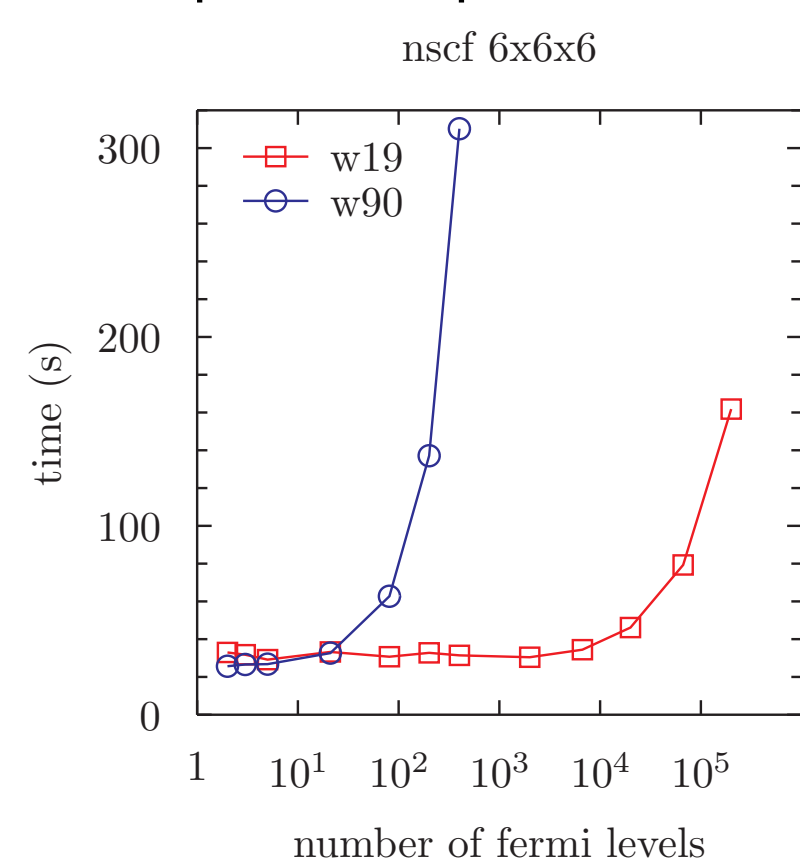
Computational time

Calculations were performed with WannierBerri and wannier90 on identical 40-core nodes of a cluster at UZH. Different grids of ab-initio (nscf) and interpolation grids were used. (**account of symmetries and adaptive refinement are switched off for w19**)



One can see that while for w19 the computational time does not depend on the ab-initio grid and the use of parameter "use_ws_distance". While for w90 they increase time a lot.

Also scanning multiple fermi levels has almost no cost in w19 up to 10^4 points:



Recursive adaptive refinement

A few k-points are chosen that give the largest contribution to the integral, or to the jittering of the curve. — typically the points near (avoided) degeneracies. They are replaced by grids of 2x2x2 points surrounding it. The procedure is repeated recursively (new points can be refined again) to get a smoother curve.

Mixed Fourier Transform

n — size of *ab initio* grid

$N = m \times n$ — size of interpolation grid (m -integer)

we want to Fourier Transform a quantity A:

$A(R_1), \dots, A(R_n) \rightarrow A(k_0), \dots, A(k_{N-1})$, where $k_i = 2\pi i/N$

For each $j = 0, \dots, m-1$ we "slow FT"

$A(R_j) \rightarrow \tilde{A}^j(R_j) = A(R_j) \times e^{2\pi i l_j^j}$

and then do a FFT of $\tilde{A}^j(R_j)$, thus getting

k-points $k_{i,j} = 2\pi(j + im)/N$

time scaling:

slow FT $\propto N \times n$

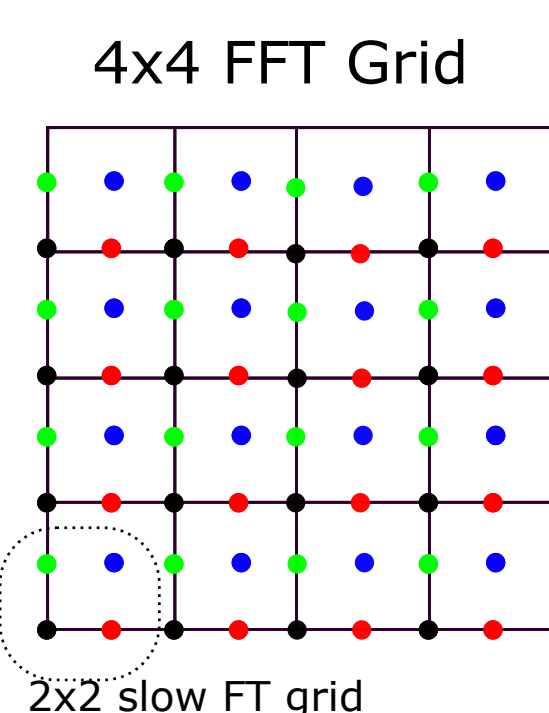
fast FT $\propto N \log N$

mixed FT $\propto N \log n$

Thus, FFT is better than SFT for large ab initio grids, while MFT is better in any case.

Advantages of mixed FT over FFT:

- ▶ easier parallelization
- ▶ allows to remove symmetry-equivalent "slow" k-point
- ▶ no need to store the whole interpolation grid (less memory needed)
- ▶ allows adaptive recursive refinement of most "important" points.



tutorial.py

```
1#!/usr/bin/env python3
2num_proc=16
3
4import wannierberri as wberri
5import numpy as np
6
7system=wberri.System(tb_file='Fe_tb.dat',getAA=True)
8SYM=wberri.symmetry
9generators=[SYM.Inversion,SYM.C4z,SYM.TimeReversal*SYM.C2x]
10
11wberri.tabulate(system,
12                NK=96,
13                quantities=["V","berry"],
14                symmetry_gen=generators,
15                fout_name="Fe",
16                numproc=num_proc,
17                Ef0=12.6,
18                restart=False)
19
20wberri.integrate(system,
21                NK=96,
22                Efermi=np.linspace(12.,13.,1001),
23                smearEf=10, # 10K
24                quantities=["ahc","dos"],#,"ahc_band"],
25                numproc=num_proc,
26                adpt_num_iter=0,
27                fout_name="Fe",
28                symmetry_gen=generators,
29                restart=False )
```

Acknowledgements

I thank Ivo Souza and Miguel Angel Jiménez Herrera for fruitful discussion