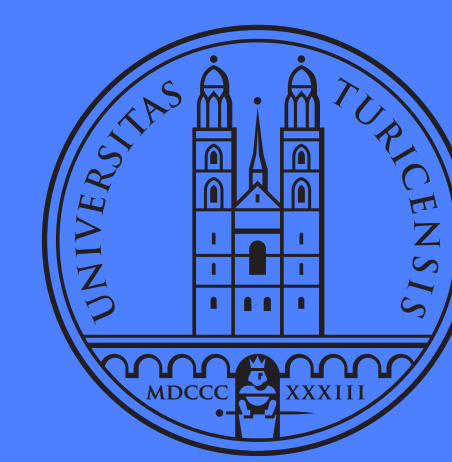




# WANNIER BERRI : an advanced tool for interpolation of Berry curvature and related quantities. (aka Wannier19)

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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:

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

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

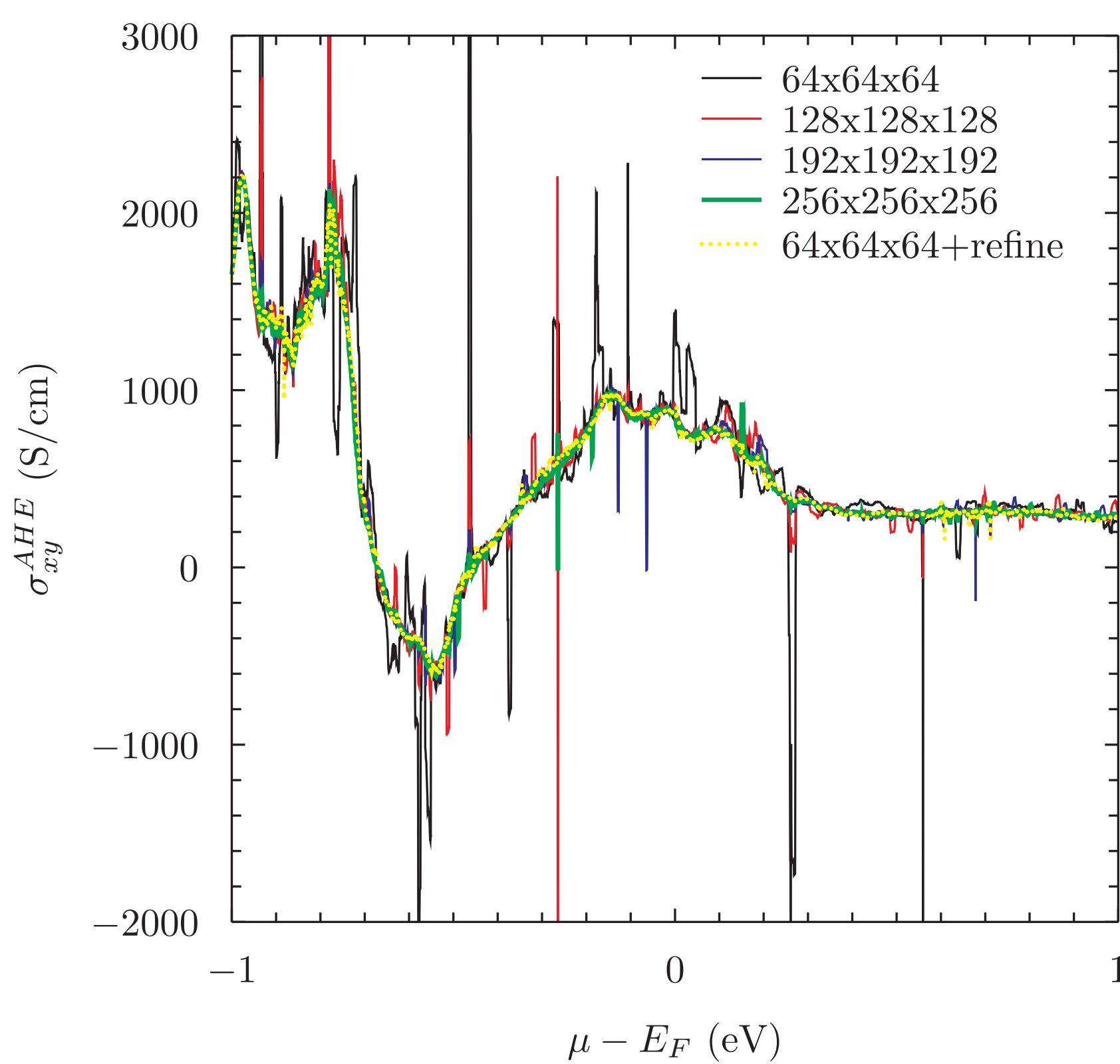
- ▶ a smooth gauge
- ▶ dense grid of  $\mathbf{k}$ -points

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  $\sigma^{\text{AHE}}$



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

## Overview

**W-BERRI** is an improved python implementation of postw90.x part of **Wannier90**. ("19-- because it was started in 2019.)

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

**Wannier90** is **good**, because it

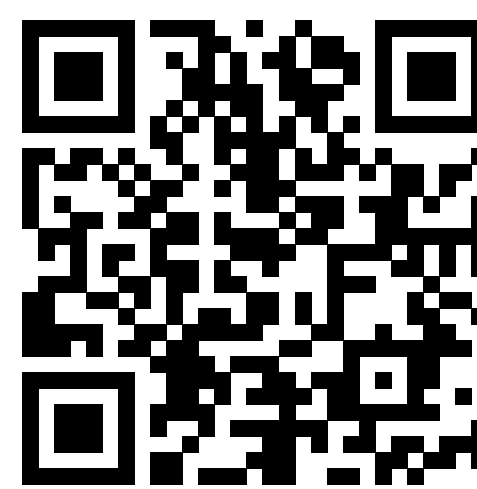
- ▶ is a well-established code
- ▶ known for ages
- ▶ has a broad community of developers
- ▶ has many implemented features
- ▶ ..... (many more)

**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>

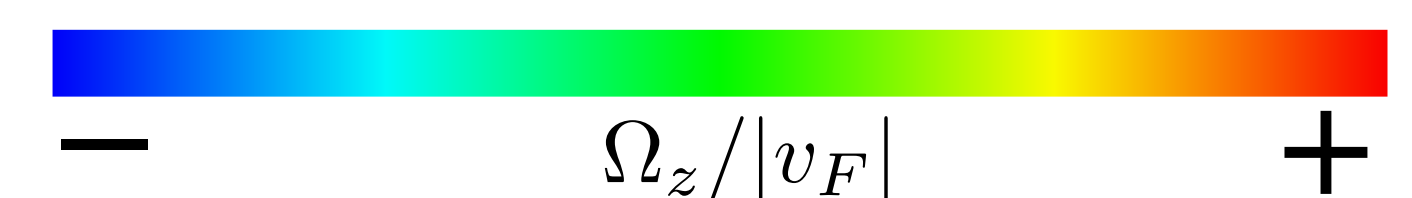
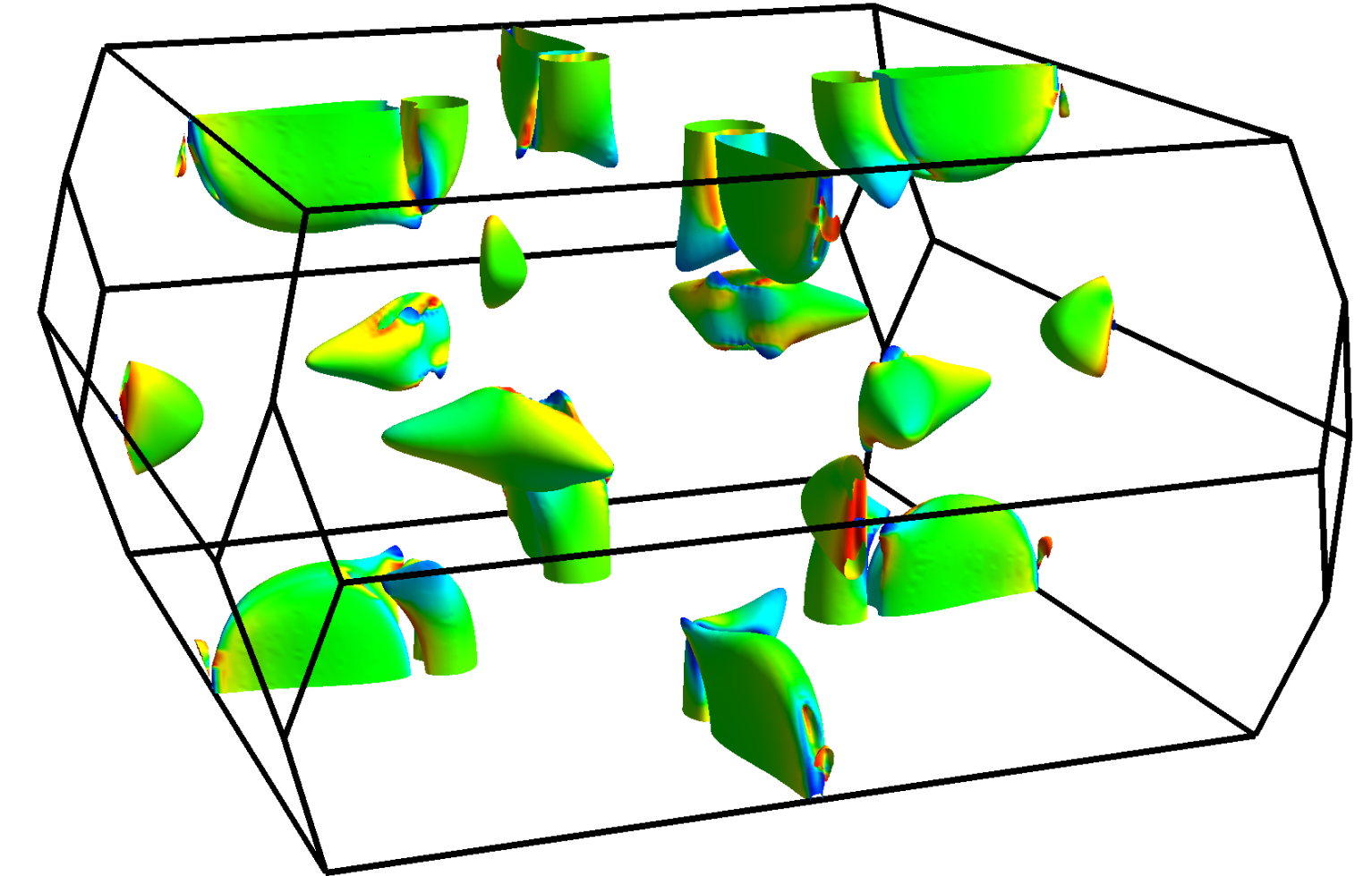


## Install with pip

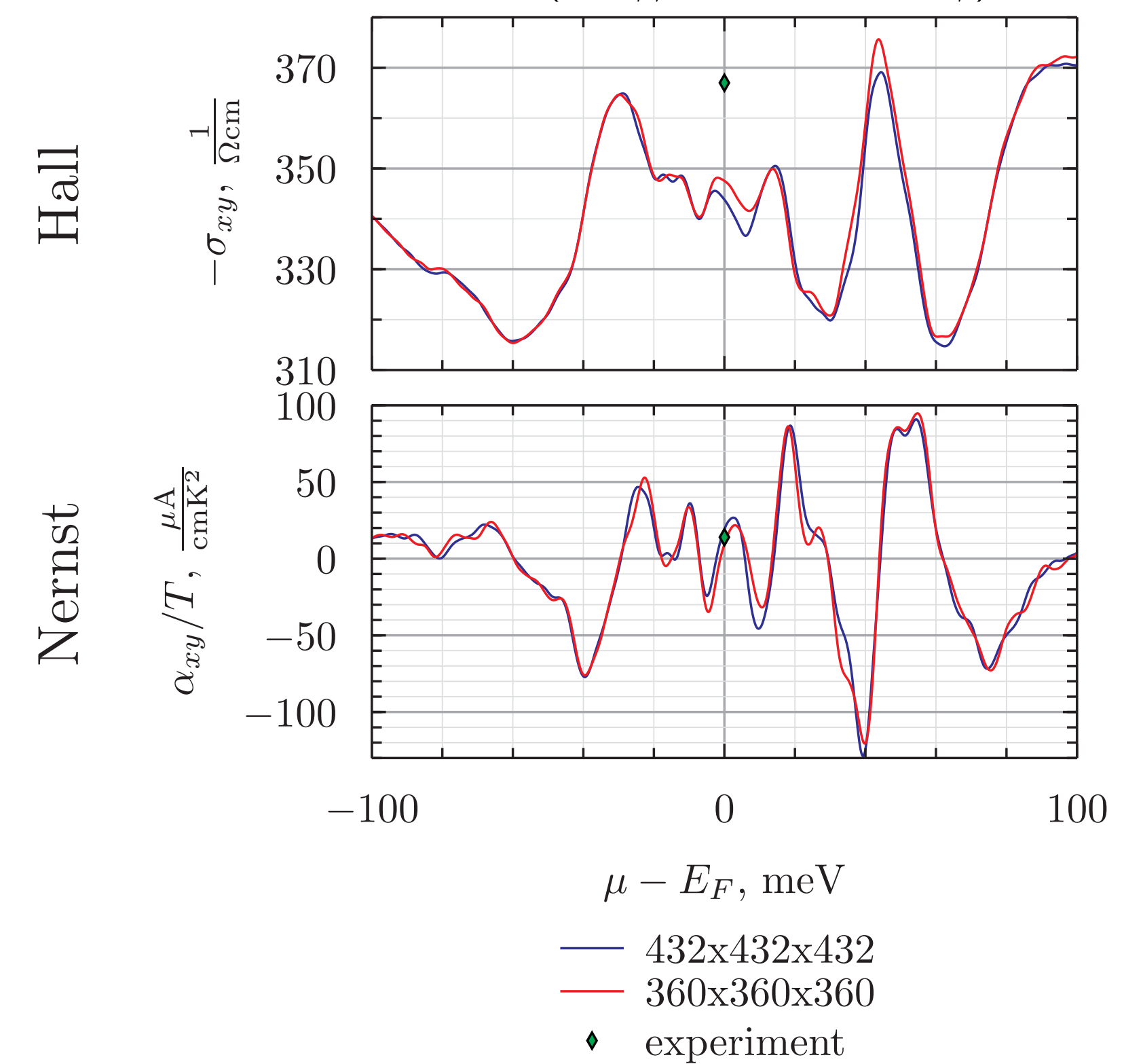
`pip3 install wannier19`

## 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**.



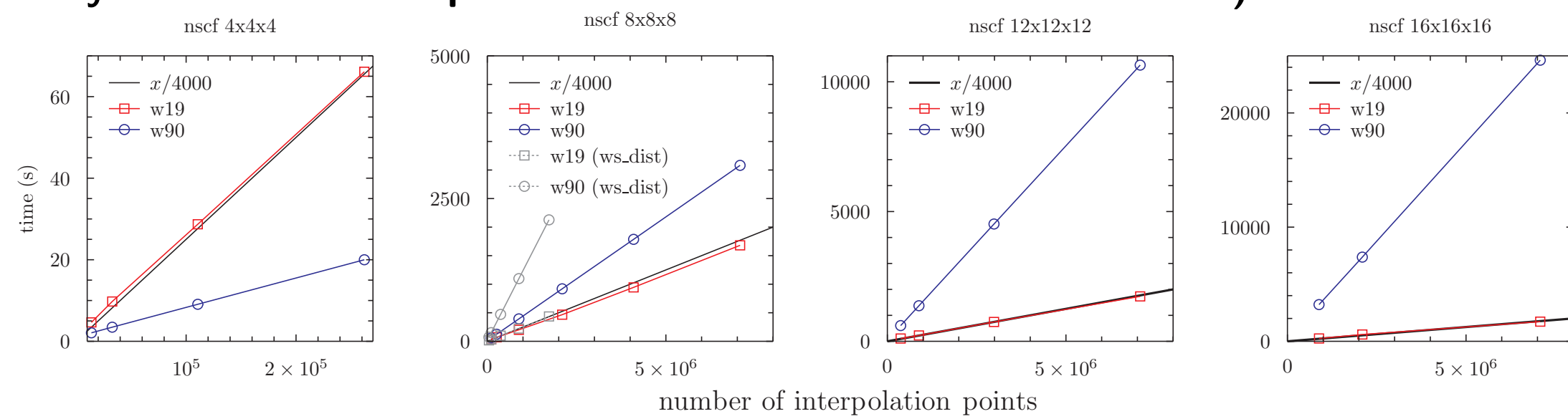
Irudia 2: Fermi surface of ReAlGe coloured by Berry curvature divided by Fermi velocity. Plot produced by FermiSurfer (<http://fermisurfer.osdn.jp/>)



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

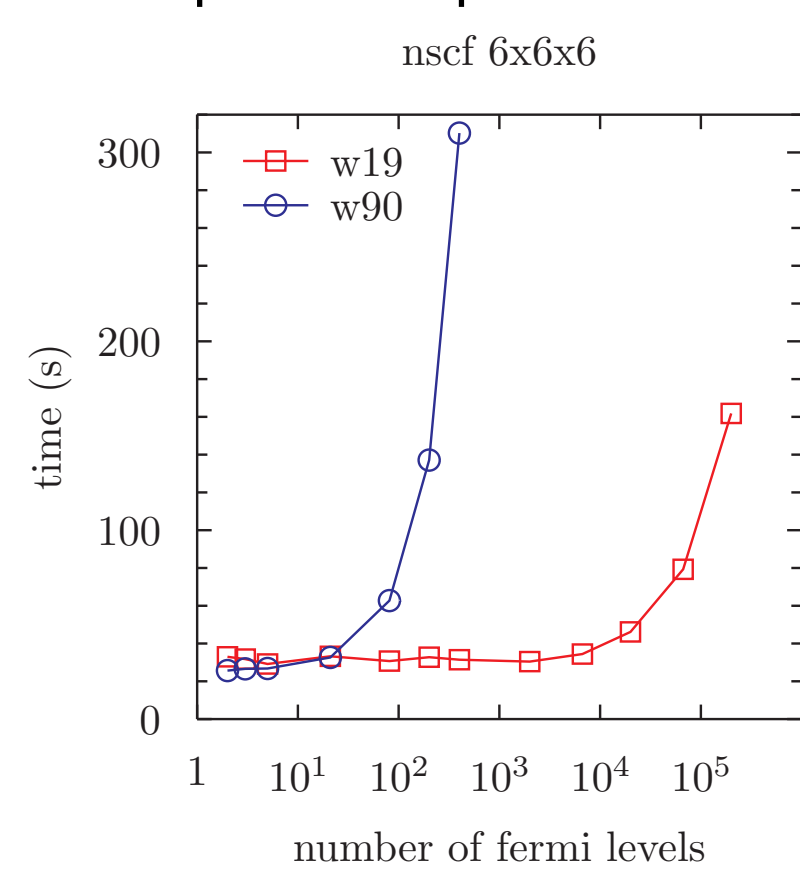
## Computational time

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  $\mathbf{k}$ -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  $2 \times 2 \times 2$  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"  
 $A(R_i) \rightarrow \tilde{A}^j(R_i) = A(R_i) \times e^{2\pi i I_j^i}$   
and then do a FFT of  $\tilde{A}^j(R_i)$ , thus getting  
 $\mathbf{k}$ -points  $k_{ij} = 2\pi(j + im)/N$

time scaling:

slow FT  $\propto N \times n$

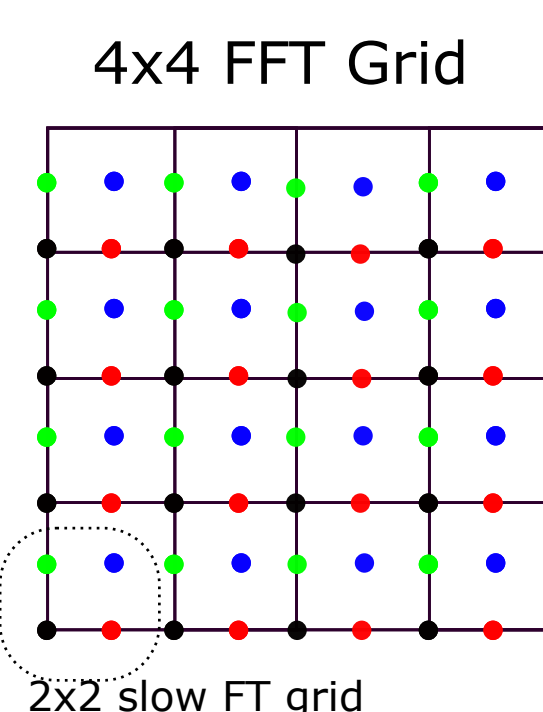
fast FT  $\propto N \log N$

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" $\mathbf{k}$ -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
2  import wannier19 as w19
3  import numpy as np
4
5  name="Fe"
6  NK=(96,96,96) # a grid 96x96x96
7  Efermi=np.linspace(12.,13.,1001) # range of Fermi levels
8  system=w19.System(tb_file='Fe_tb.dat',getAA=True)
9
10 # symmetries of the system to be accounted for :
11 SYM=w19.symmetry
12 generators=[SYM.Inversion,SYM.C4z,SYM.TimeReversal*SYM.C2x]
13
14 # tabulate quantities to be plotted by FermiSurfer
15 w19.tabulate(system,
16             NK=NK,
17             quantities=["V","berry"],
18             symmetry_gen=generators,
19             fout_name=name,
20             numproc=4,
21             Ef0=0,
22             restart=False )
23
24 # integrated quantities
25 w19.integrate(system,
26             NK=NK,
27             Efermi=Efermi,
28             smearEf=10,
29             quantities=["ahc","dos"],
30             numproc=4,
31             adpt_num_iter=10,
32             fout_name=name,
33             symmetry_gen=generators,
34             restart=False )
```

## Acknowledgements

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