Calculation of the Maximally Localized Wannier Functions in the SIRIUS Library

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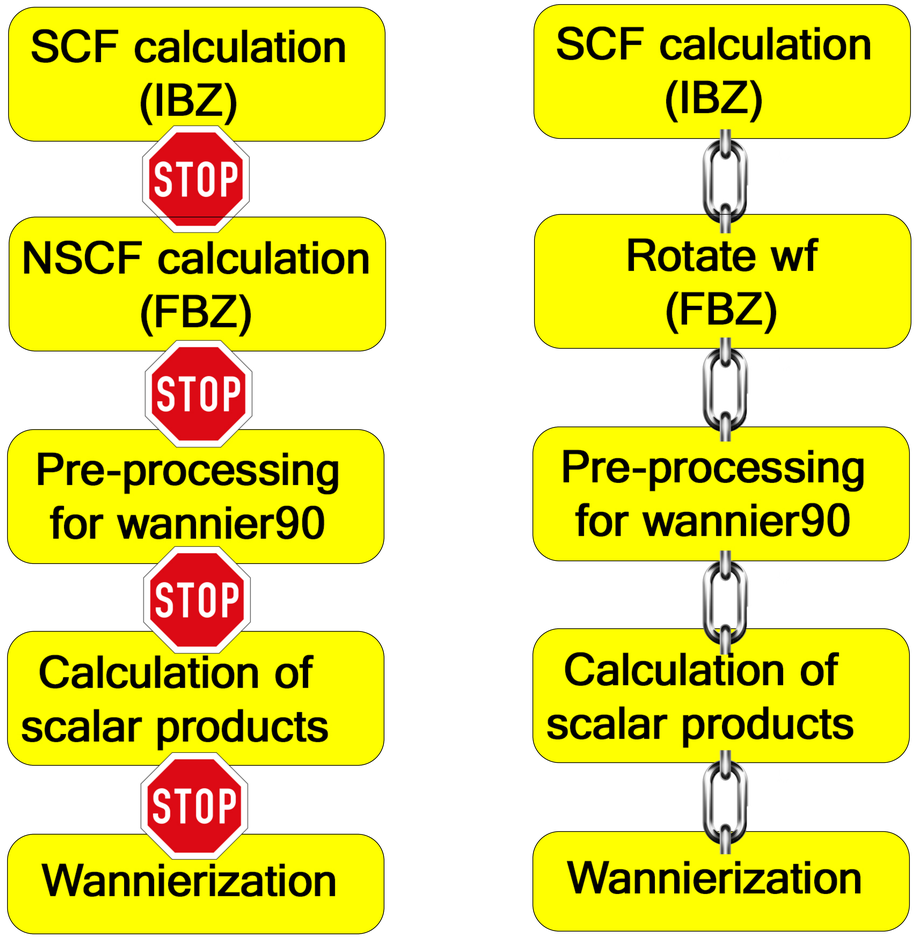
Introduction

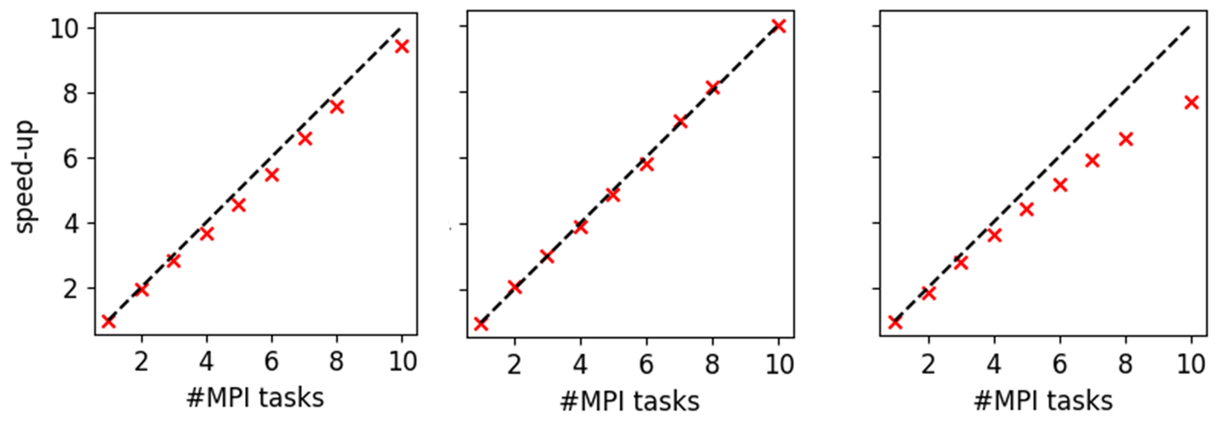
DFT+U and Koopman spectral functionals are some approaches that can correct DFT band structures, key ingredients for the understanding of electronic properties of materials. Both of them can be computed using Maximally Localized Wannier Functions (MLWF). In this work we show how the computation of MLWF has been optimized using the SIRIUS library, which streamlines linear algebra routines of DFT codes.

Algorithms in comparison

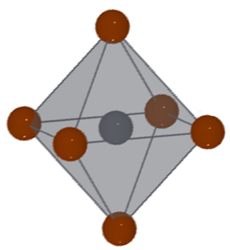


K parallelization: speed up

$\psi_{n,R\bar{\mathbf{k}}}(\mathbf{r}) = \psi_{n,\bar{\mathbf{k}}}(R^{-1}(\mathbf{r}-\boldsymbol{\tau}))$ $A^{\mathbf{k}}_{mn} = \langle\psi_{m\mathbf{k}}|w^{(0)}_n\rangle$ $M^{\mathbf{k},\mathbf{b}}_{mn} = \langle\psi_{m\mathbf{k}}|e^{-i\mathbf{b}\cdot\mathbf{r}}|\psi_{n,\mathbf{k}+\mathbf{b}}\rangle$



Benchmark run: $CsPbBr_3$



→ 20 atoms per unit cell
→ 104 wannier orbitals
→ 260 bands
→ 1k plane waves
→ 144 k points

Time comparison for matrix elements

Running on 10 nodes on CPUs
Intel® Xeon® E5-2690 v3 @ 2.60GHz

Time SIRIUS:	459.35 s
Time QE:	953.85 s

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