# SiScLab Project 8

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January 24, 2019

# Problem Statement

- Solid state physics: electronic structure computation
  - $\rightarrow$ Fleur: electronic structure of crystals using DFT
  - huge amount of data
  - physics not accessible unless structured / analysed / visualized

The goal of the project was to implement a complete data analysis pipeline for this application:

- preprocessing $\rightarrow$ data exploration $\rightarrow$ visualization

# Motivation

- Physicists problem with the simulation data
- fast computation time
- code modularization
- intuitive usage
- high-quality export features

# Requirements

- process Fleur output files
- fast computation
- code: modularization, easy maintainability
- frontend: no installation required, intuitive usage
- plots: publication-quality export

# Steps

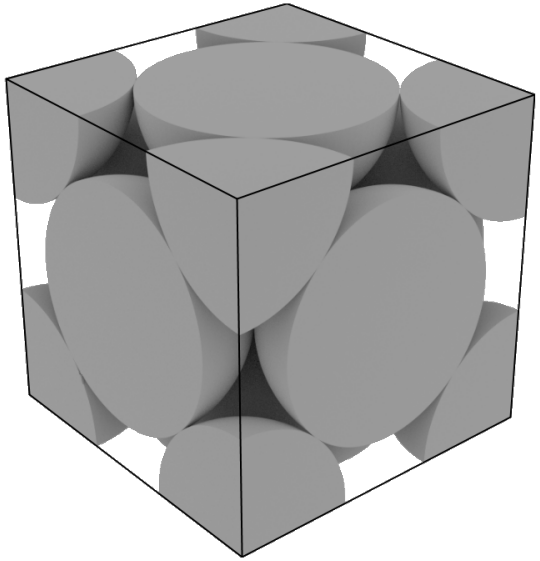
- Understanding physics and problem
- preprocessing the data
- exploring the data(implementation)
- visualization(GUI)
- Results

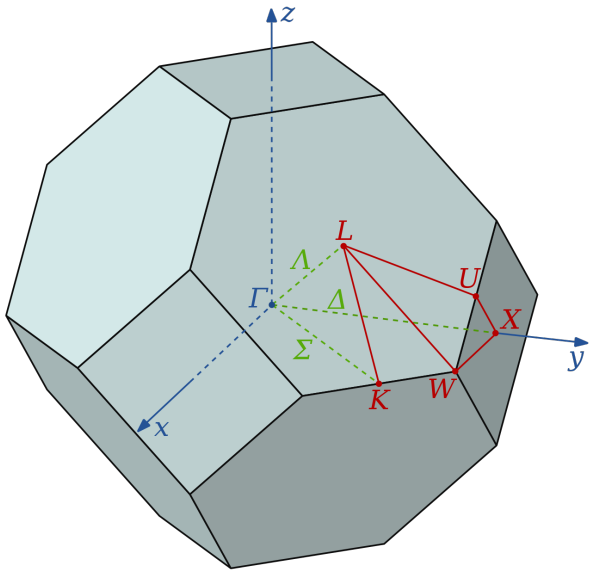
# How is the data generated?

- Fluer computes electron density in crystals
- Density functional theory (DFT) approach:
  - Hohenberg Kohn theorem: use electron density
  - Kohn Sham system: Solve one particle Schrödinger equations in effective potential (self consistent)
  - State of the art method for electronic structure computations in solids

# What data is generated?

- Bandstructure $E_\nu(k)$:
  - Eigenenergies of (Bloch-) Eigenfunctions of the Hamiltonian for each (crystal-) momentum $k$
  - Disperion relation: Relation between crystal momentum and Energies of the Bloch electrons
  - Sampled along a 1d Path between high symmetry points in 3d reciprocal space

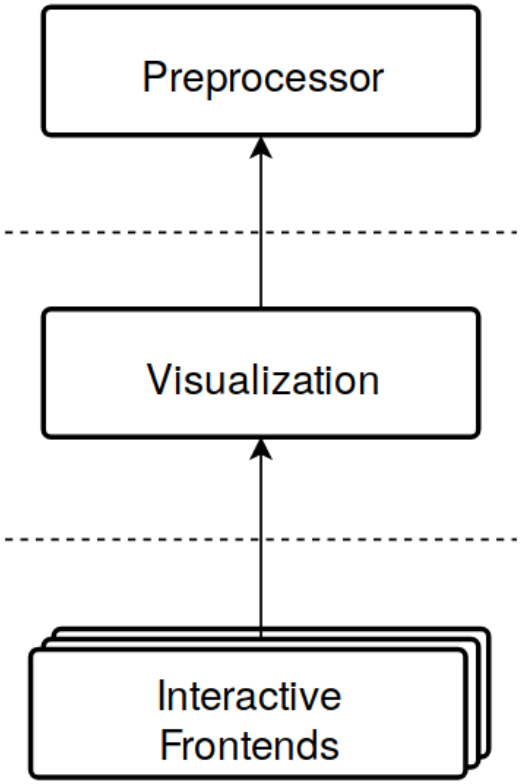




- Bandstructure D(E):
  - Density of electron states per energy interval

- Interesting for Physicist: Where do the contributions to E(k) and D(E) come from?
  - Contributions from Basis functions of the DFT calculation corresponding to different Atomgroups and atomic orbitals (s, p, d, f)
  - User might be interested in any superposition of them (e.g. to locate states in real space)
  - Information stored in form of weights for all Atom Groups and the atomic orbitals s, p, d, f

# Module Design Goals




Multifunctionality:

- automated workflows like in AiiDA
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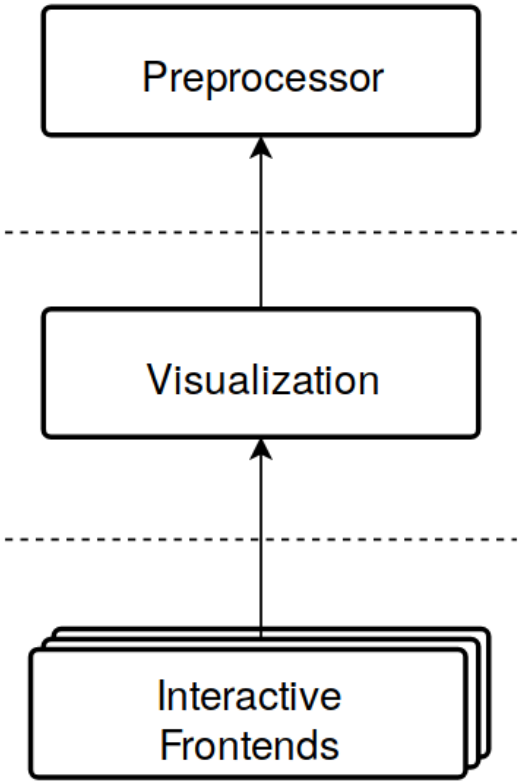


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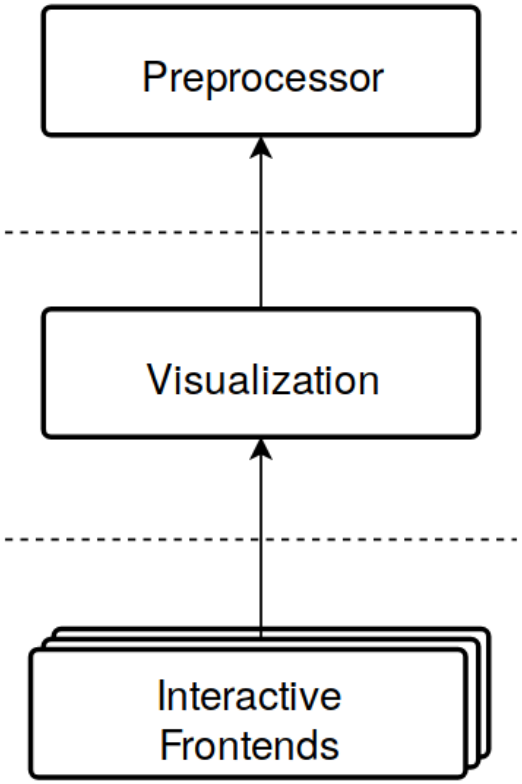


Multifunctionality:

- automated workflows like in AiiDA
- manual data analysis with Python

- no boilerplate code!

- Desktop
- Web → like in AiiDAlab

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Input: Fleur calculation results stored in Hierarchical Data Format (HDF).

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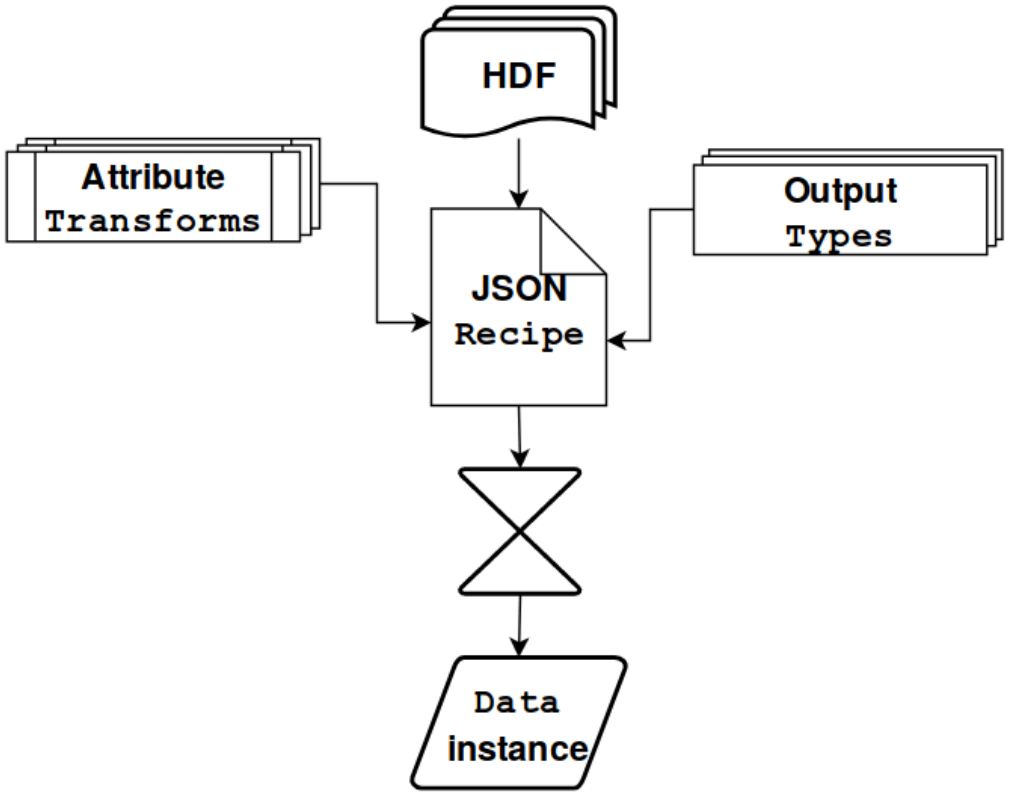


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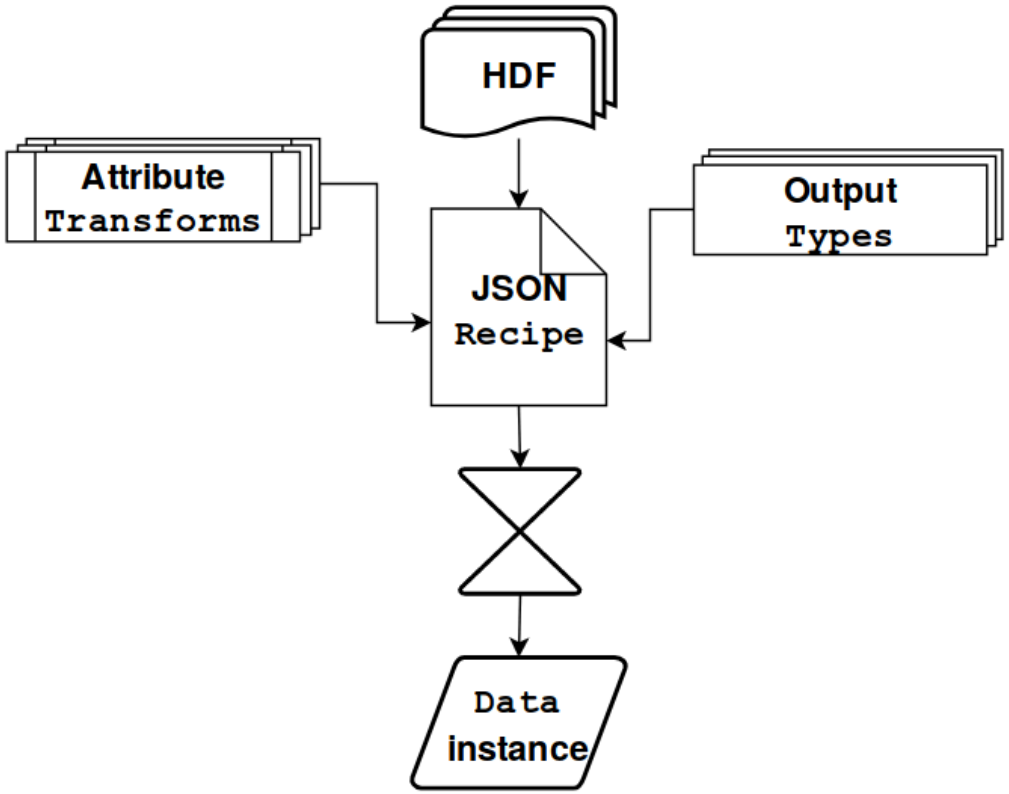


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# Data Selection for Viz

The main compute-intensive routine:

$$W^{\text{eff}}_{s,\mathbf{k},\nu} = \left( \frac{\sum\limits_{\substack{g \in \text{groups} \\ c \in \text{characters}}} n_{s,\mathbf{k},\nu,g,l} N_g}{\sum\limits_{\substack{g \in \text{all groups} \\ c \in \text{all characters}}} n_{s,\mathbf{k},\nu,g,l} N_g} \right) \left( W^{\text{unf}}_{s,\mathbf{k},\nu} \right)^{\alpha}$$

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Optimizations:

- reshaping $(\mathbf{k}, \nu) \rightarrow (\mathbf{k} \cdot \nu)$
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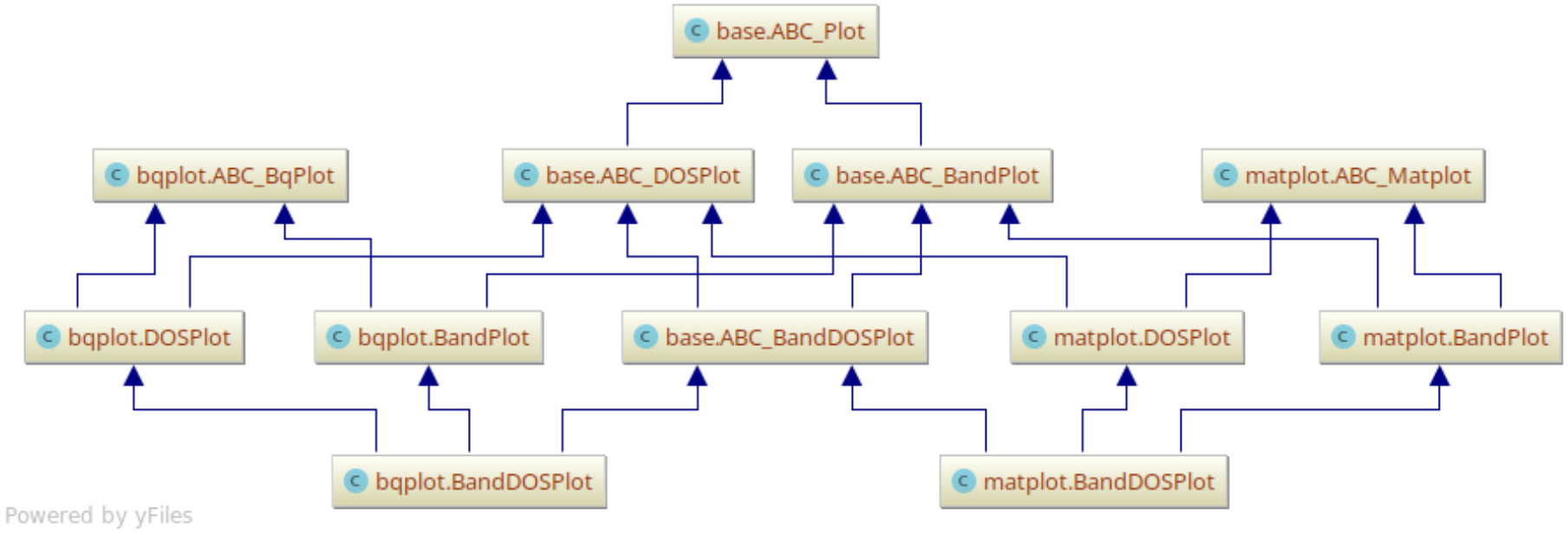

# Desktop Frontend

Choice of GUI Toolkit: **TKinter**, Kivy, PySide/PyQt, ...
Choice of Plotting tool: **matplotlib**

# Web Frontend

The Python Visualization Landscape as of 2017...

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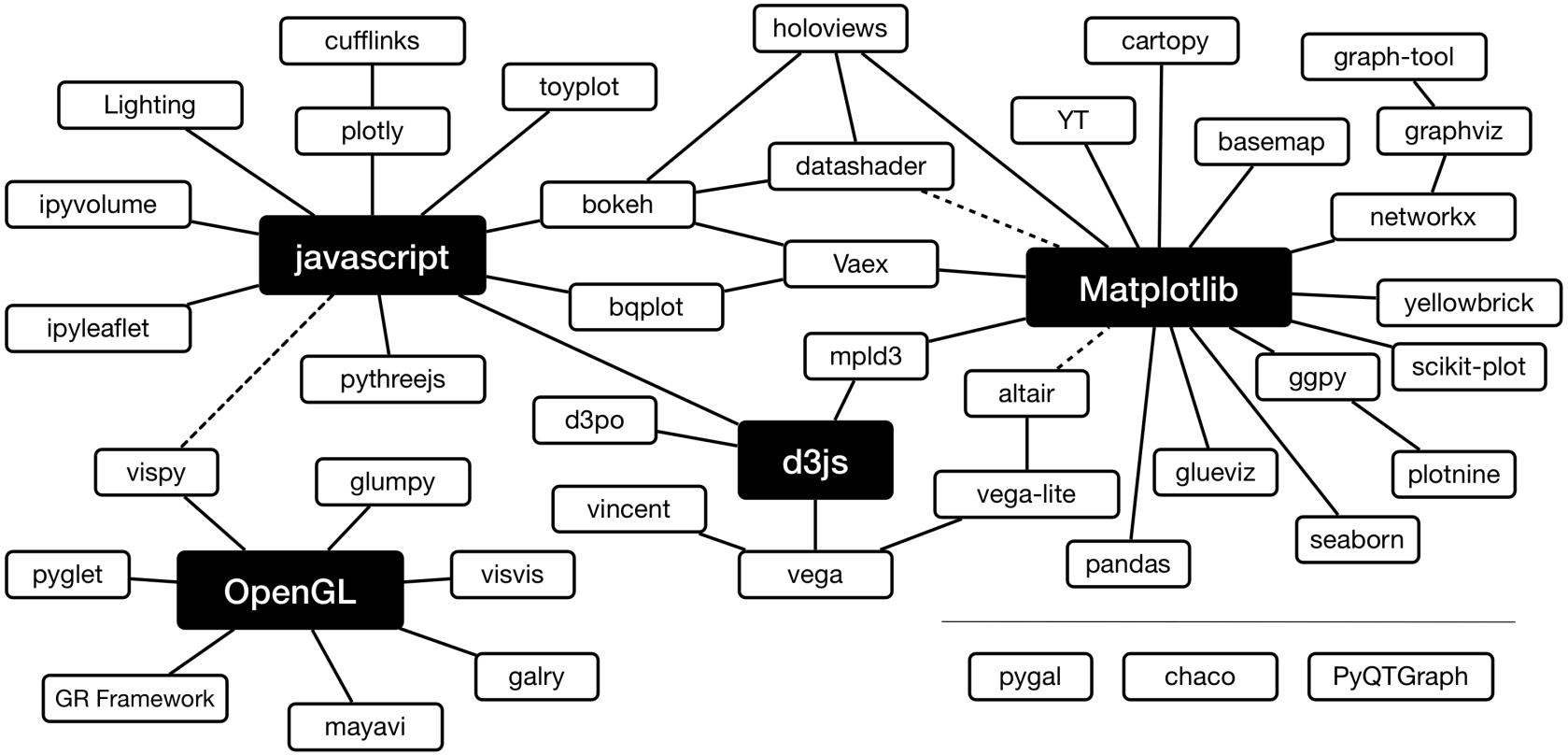


Python Visualization Landscape by rougier / BSD-2

# Web Frontend

- Needed: an OSS **Tool Selection Process** for building a Web Dashboard using **only** .
- Decision Priority Order: *support...*
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| III. **Plots**[3] | | | | |
| - 2D | mpl, bqplot, ... | hvplot, Bokeh | Bokeh | plotly |
| - 3D | ipyvolume | ✖ | Bokeh | plotly |

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# Effective mass and Fermi velocity:

- Derived Quantities:
- mass, that an electon in a crystal appears to have compared to a free electron (due to interactions in the solid)
- $m^* = \hbar^2 \frac{d^2 E(k)}{dk^2}$
- Group velocity at the Fermi energy
- $v_{Fermi} = \frac{dE(k)}{dk}$ at $E = E_F$
- Bandstructure periodic: Using FFT to compute accurate Derivates:
- $\Leftrightarrow$ Differentiate finite Fourier Series $f^{(n)}(x) = \mathcal{F}^{-1}\left((ik)^n \mathcal{F}(f(x))\right)$