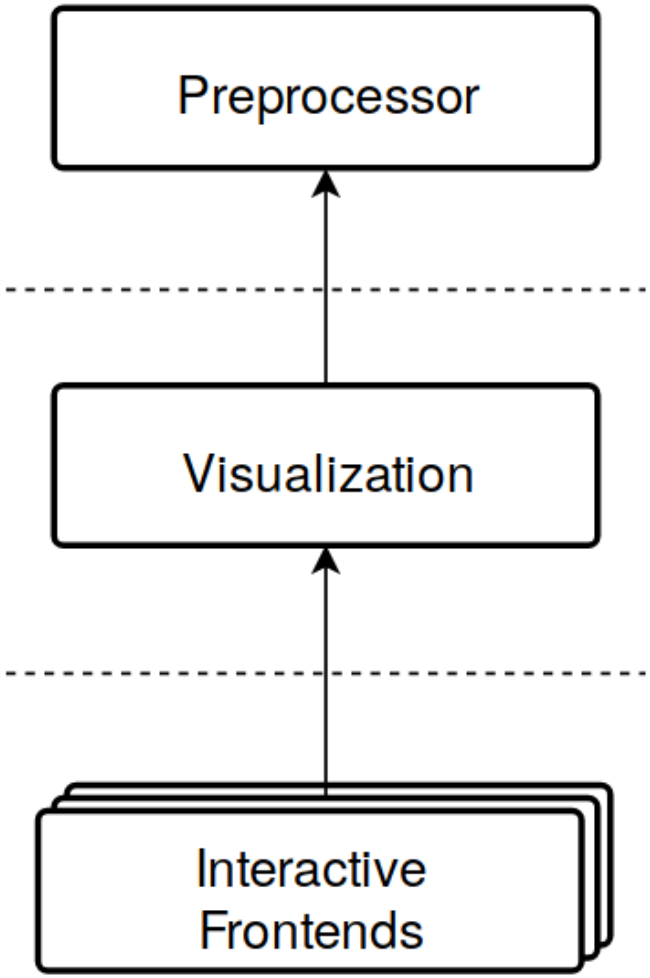
Module Design

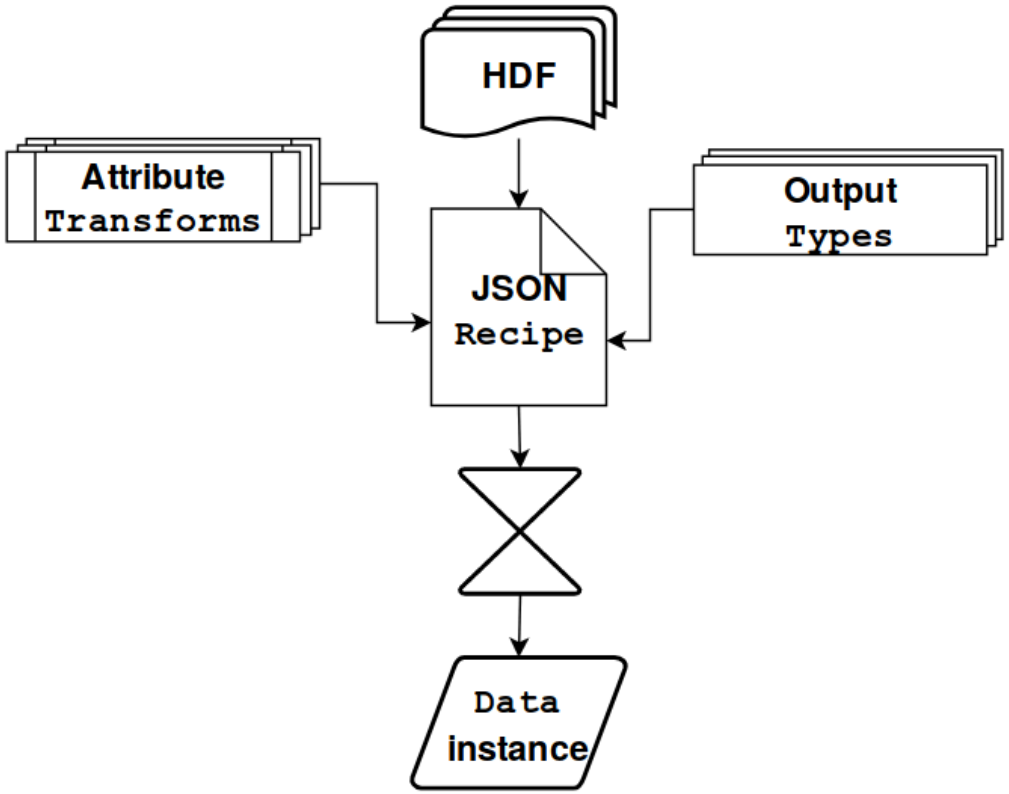


- usable in automated workflows like in AiiDA

- one code for all

- for Desktop
- for Web like in AiiDAlab

Preprocessor Module



Input: Hierarchical Data Format (HDF).
Module uses type introspection to enable features:

- modular output types
- dependency resolution

Data Selection

l-like charge density: $n^{\mu}_{\nu,l}(\mathbf{k}) = \int_{MT^{\mu}} |\psi^{\mu}_{\nu,l}(\mathbf{k},\mathbf{r})| d^3r :\approx L_{skngc}$
The main compute-intensive routine:

$$W^{\text{eff}}_{s,\mathbf{k},\nu} = \left(\frac{\sum_{\substack{g \in \text{groups} \\ c \in \text{characters}}} L_{s,\mathbf{k},\nu,g,c} G_g}{\sum_{\substack{g \in \text{all groups} \\ c \in \text{all characters}}} L_{s,\mathbf{k},\nu,g,c} G_g} \right) \left(W^{\text{unf}}_{s,\mathbf{k},\nu} \right)^{\alpha}$$

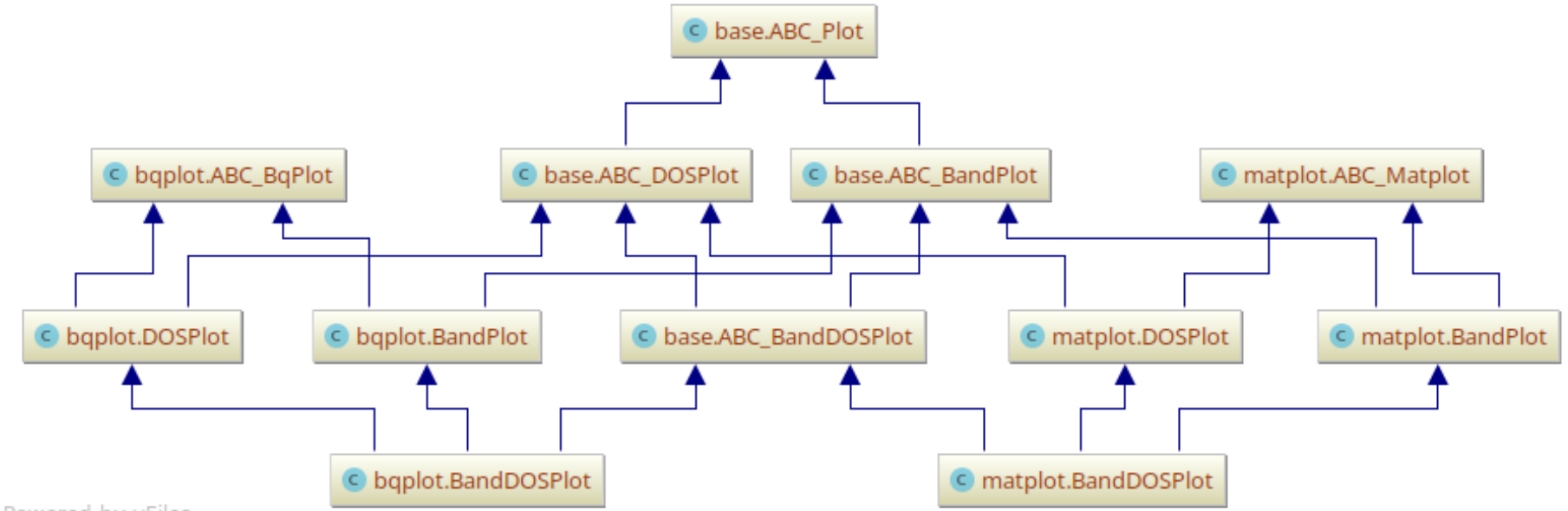
Optimization

- reshaping $(\mathbf{k}, \nu) \rightarrow (\mathbf{k} \cdot \nu$
- weight filter t: $W^{\text{eff}}_{s,\mathbf{k},\nu} > t$
- TODO ??? `np.tensor` ???
- buffering on selection change

TODO Result: speedup of about ???factor???

Visualization Module

- Abstract interfaces for different viz. libs and applications
- `InteractiveControlDisplay` as frontend contracts



Desktop Frontend

TODO Praneeth?

Web Frontend

TODO Selection Process from Notes

TODO Selection Process Choices from Notes