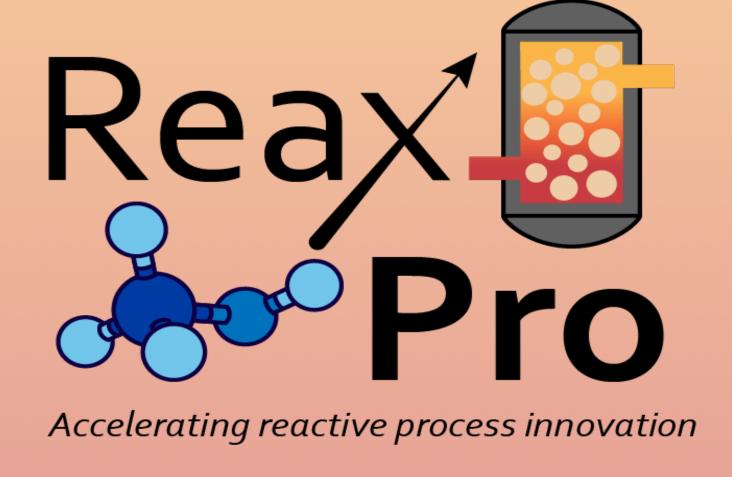
Pablo Lopez-Tarifa Netherlands eScience Center

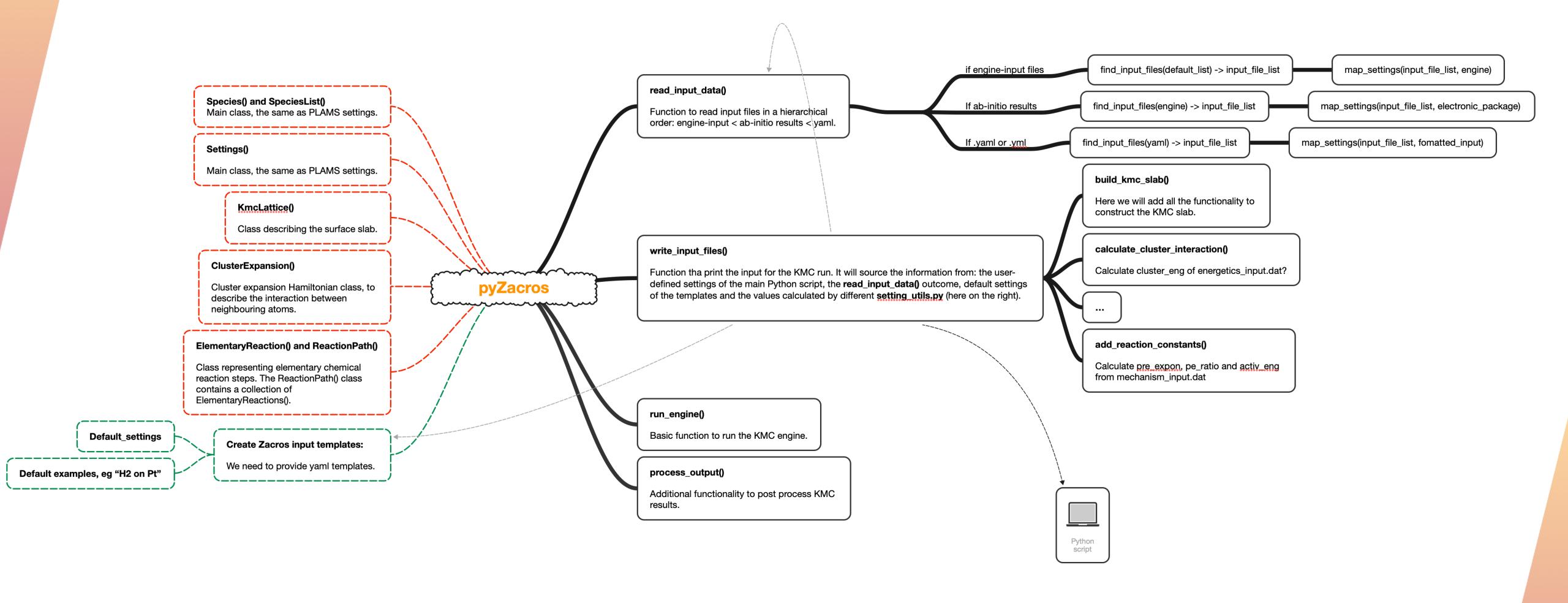


pyZacros

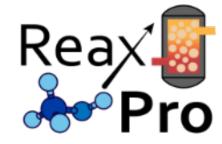




pyZacros skeleton

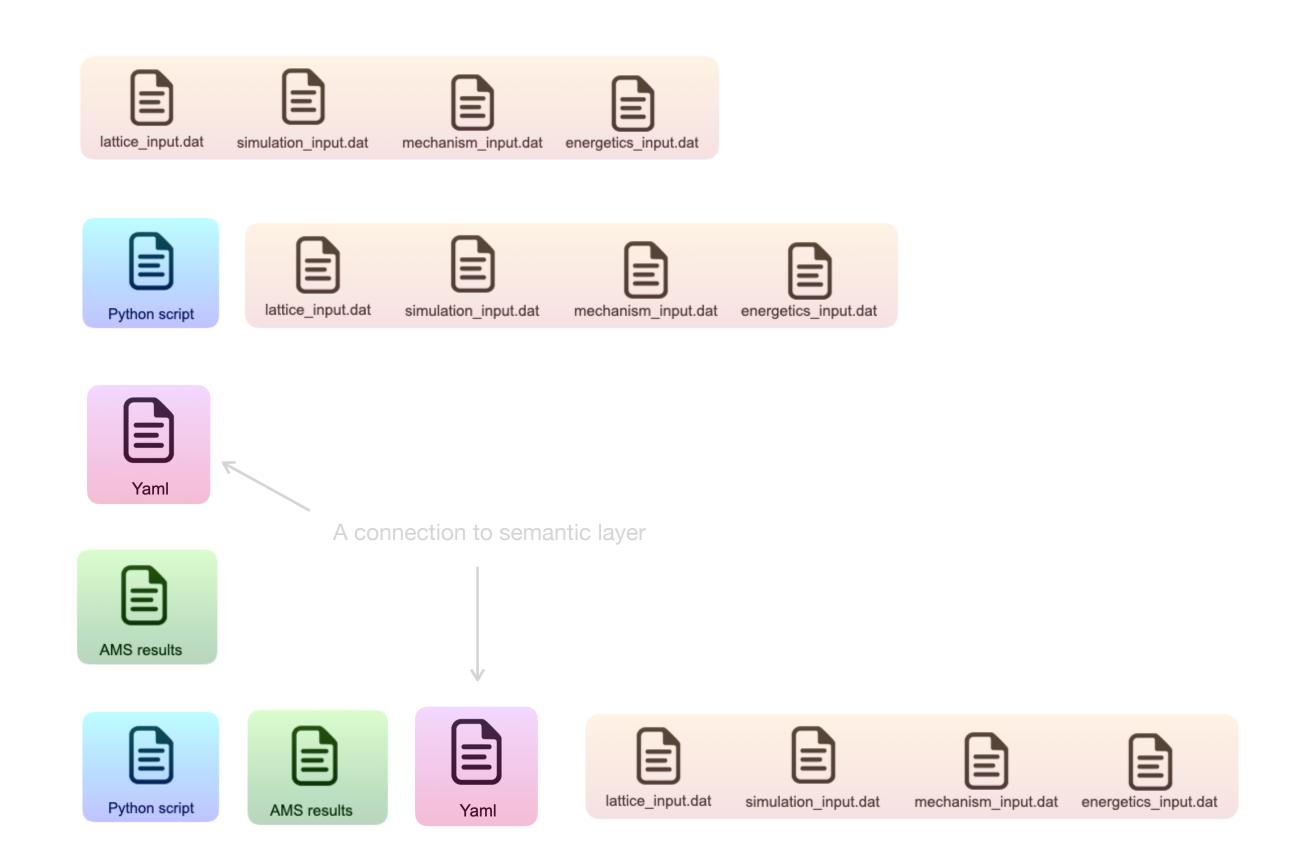






pyZacros: Possible read input scenarios

- 1. All Zacros input files, nothing to do:
- 2. Some settings are provided in the Python script:
- 3. Zacros inputs are provided using Yaml format:
- 4. Inputs are built from ab-initio outputs:
- 5. A bit of everything:







Level 2: Connection with OSP/EMMO ontology

A CWL workflow will open a wrapper sessions for each of the engines. Data will be transferred using CUDS objets.

