ISPyB Status at DESY

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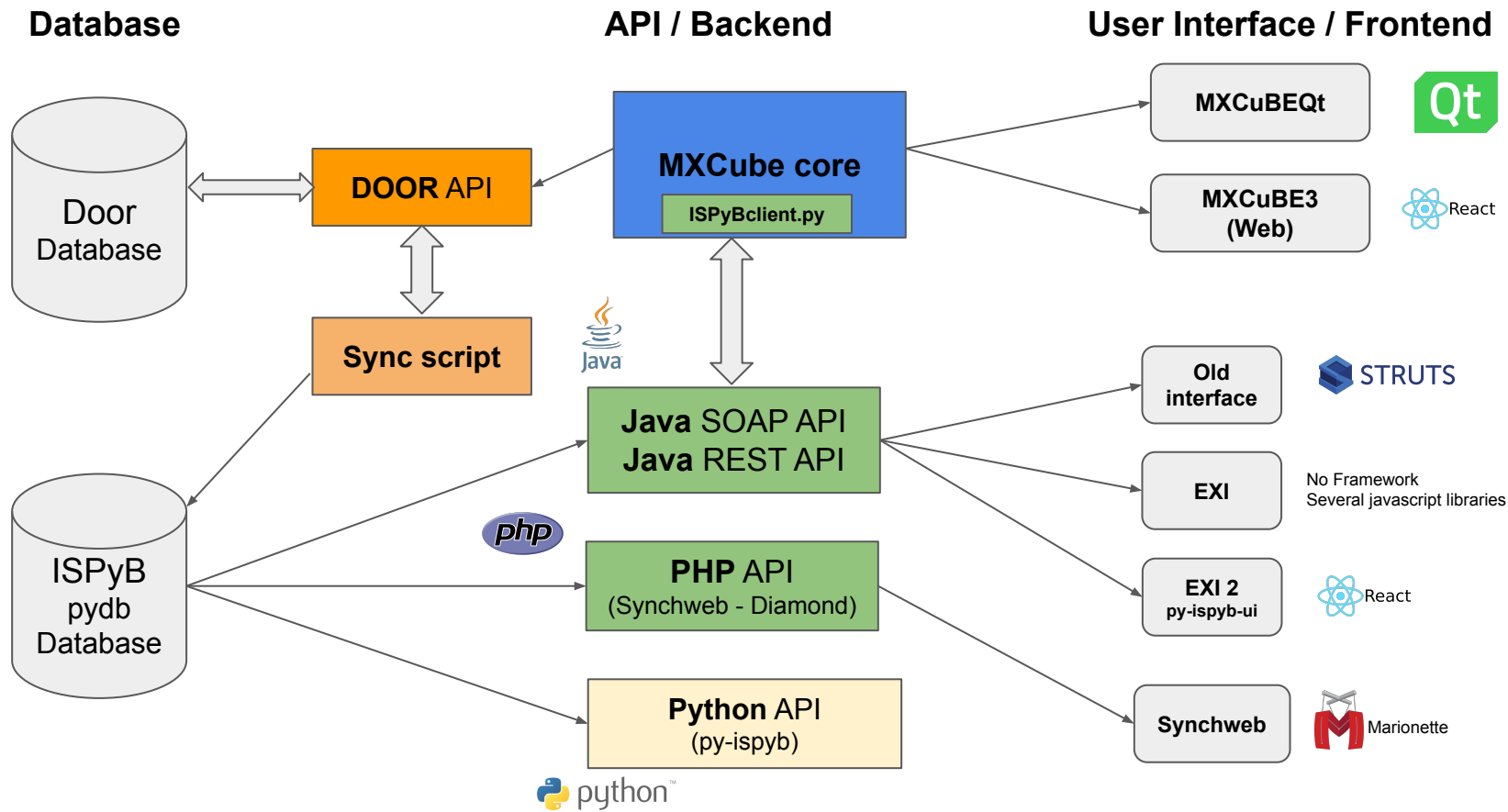
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Background

- Started with ISPyB at DESY in January 2022

- MXCuBE currently been implemented but it is not ready yet
  - New Software Control engineer (Andrey Gruzinov) since May 2022
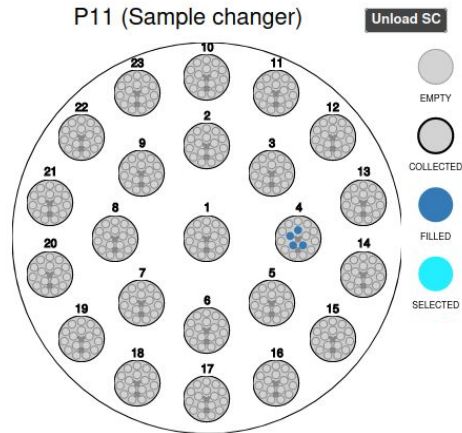 - Currently an in-house data acquisition software is in place

ISPyB at DESY

- We have currently a testing server with the ISPyB JAVA API together with EXI as frontend:

  - https://ispybdev.desy.de
  - https://exidev.desy.de

- Changes done to adapt ISPyB JAVA API to DESY:
  - ISPyB DESY profile
  - Custom authentication module
    - Authenticate against DOOR
  - Minor adaptations for DESY

- Changes done to EXI
  - Minor user interface adaptations
  - Minor EXI configurations for DESY
  - Custom Sample Changer widget
    - To be migrated to py-ispyb-ui

Current focus

- Our focus now is to synchronize User portal proposals and sessions into the ISPyB database
  - Tested already with an legacy python client
    - https://github.com/ispyb/ispyb-client/tree/master/python/userportal
  - Being discussed/implemented in py-ispyb

- DESY has develop a new API to get proposals, sessions, etc from the user portal (DOOR)
  - A python package has been created as a wrapper to convert the data to any desired structure

- py-ispyb User portal synchronization module (Working group)
  - Common data-ingestion input format to be used to import data into ISPyB (based on JSON)
    - To be agreed
  - Advantage of defining common data-ingestion input format/structure
    - py-ispyb user portal sync module may be used by all parties
    - Possibility to add automatic testings
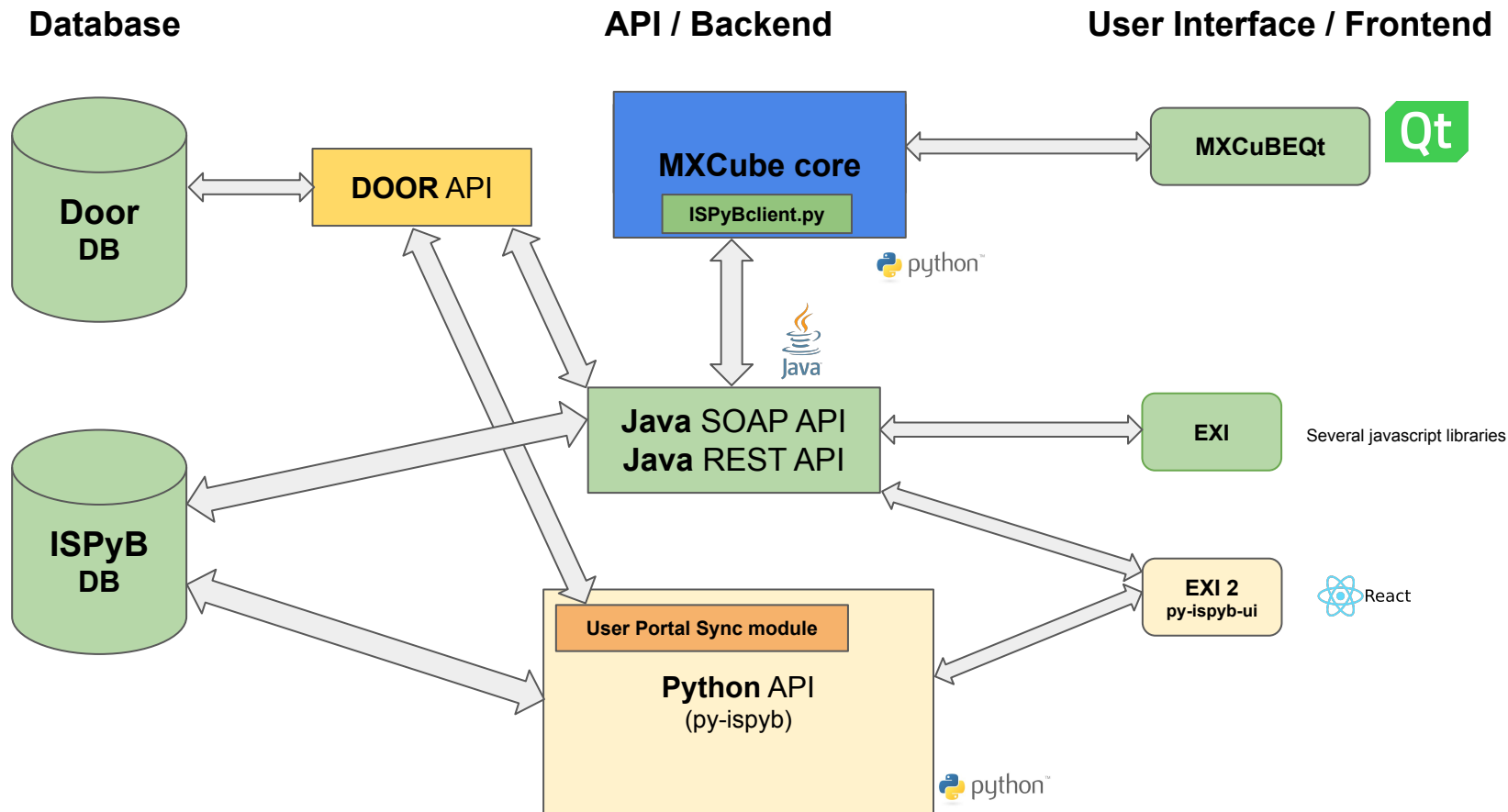
py-ispyb User Portal Sync

- Define the common data-ingestion input structure
    - Create pydantic models automatically from sqlalchemy models
        - https://github.com/tiangolo/pydantic-sqlalchemy

    - From the pydantic models one can create a json-schema to validate the input data
        - UserPortalSync.schema_json(indent=2)

    - The generated json-schema will be accessible from a py-ispyb endpoint
        - Any facility will be able to validate their User Portal data against the defined json-schema
        - Each facility will need to adapt their data according to the json-schema
        - The schema will follow the ISPyB DB structure

Roadmap

- Plan A (depending on how fast we have MXCuBE ready)
  - API: go to production as soon as possible with Java API
    - Using the MXCuBE ISPyB client to communicate with ISPyB JAVA API
      - Read samples
      - Write data collections
  - User Interface: EXI
  - Implemented and tested already in several facilities
  - Slower transition to py-ispyb / py-ispyb-ui

- Plan B
  - API 1: Go to production with the JAVA API (for MXCuBE)
  - API 2: py-ispyb
  - User Interface: EXI / py-ispyb-ui

Door / ISPyB / MXCuBE - May 2022

Database

API / Backend

User Interface / Frontend

Door DB

DOOR API

MXCube core

ISPyBclient.py

MXCuBEQt

Qt

python

Java

Java SOAP API
Java REST API

EXI

Several javascript libraries

ISPyB DB

User Portal Sync module

Python API
(py-ispyb)

EXI 2
py-ispyb-ui

React

python

Thank you!