py-ispyb and ssx

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Content

- ISPyB backend server pyispyb.
- Latest developments.
- SSX data model and ssx microservice.

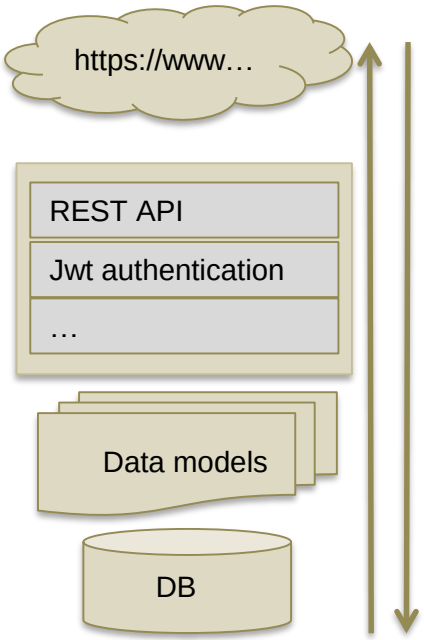
Overview

- **Python 3.x**
- **Flask**>=1.1,<2
- **flask-restx**
- Flask-Cors>=3.0.8,<4

- **SQLAlchemy**>=1.3.0,<2
- Flask-SQLAlchemy>=2.4,<3

- **marshmallow**>=2.13.5,<3
- flask-marshmallow>=0.7,<0.8
- marshmallow-sqlalchemy>=0.12,<0.13
- marshmallow_jsonschema

- **pyjwt**
- ruamel.yaml
- pdfkit
- python-barcode



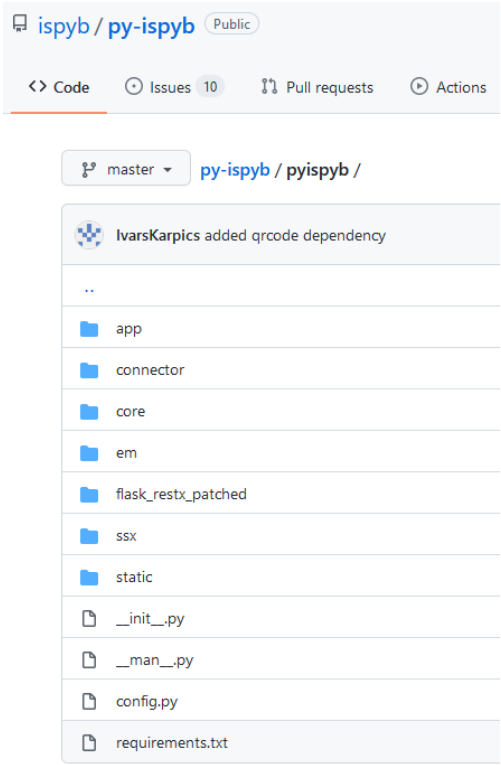
Structure

- Plug-in **extensions**: api, auth, db, logging.
- Microservice definition directories:
  - core
  - ssx
  - em

Each service contains:

- **models.py**: sqlalchemy classes reflecting the data base.
- **schemas**: flask, marshmallow and json schemas.
- **modules**: data handling modules.
- **routes**: API end point definitions.

- Scripts, tests, deploy, docker, setup.py



Versioning and deployment

1. Install pyispyb:

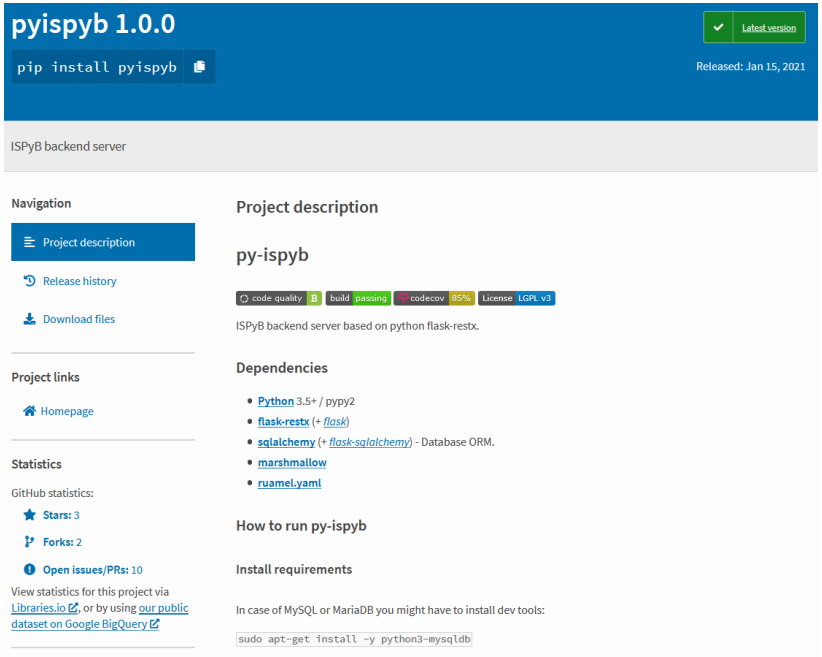
```
pip install pyispyb
```

2. Run scripts to generate data models and schemas:

```
scripts/generate_core_models.sh path_to_config_file.yml
scripts/generate_core_schemas.py
```

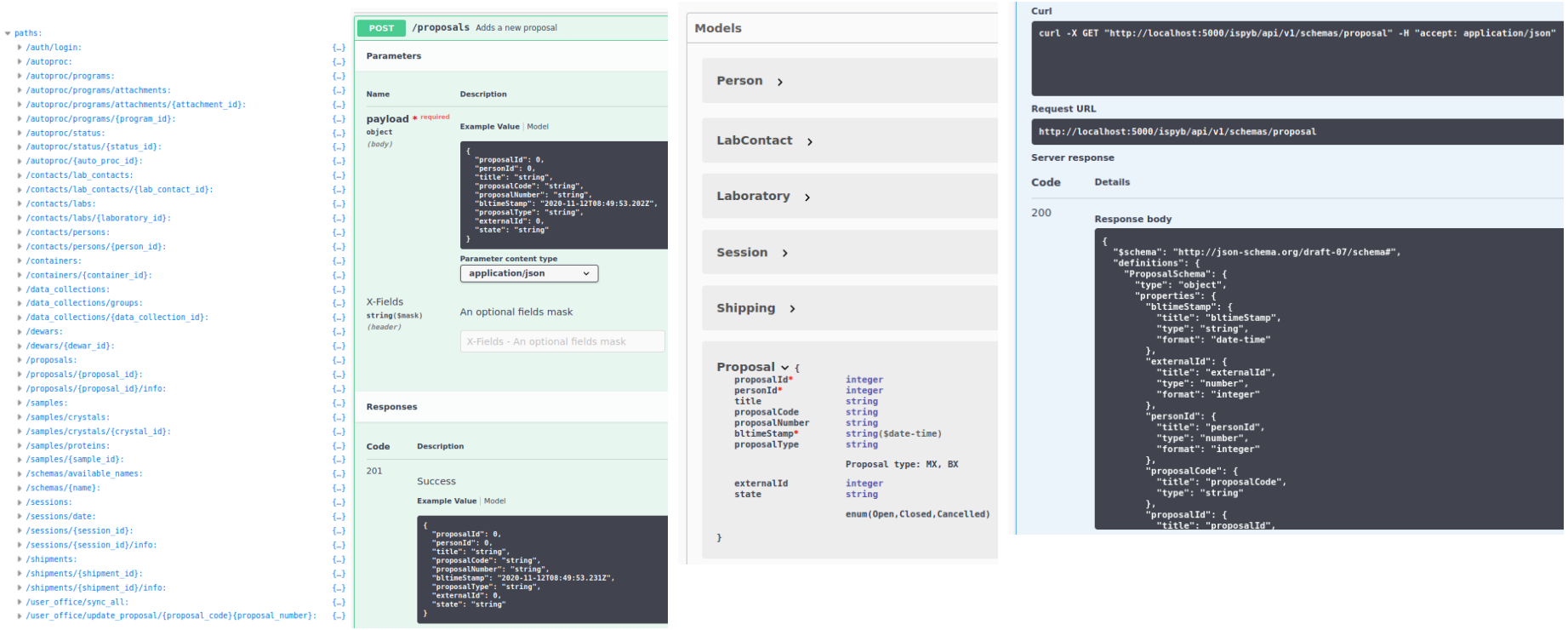
3. Start the pyispyb server:

```
from pyispyb import create_app
ispyb_app = create_app(config_filename, 'dev')
ispyb_app.run(host='0.0.0.0', port=5000, debug=True)

gunicorn -b 127.0.0.0:4000 "app:create_app()"

from gevent.pywsgi import WSGIServer
from pyispyb import create_app
ispyb_app = create_app(config_filename, 'dev')
ispyb_server = WSGIServer(('', 5000), ispyb_app)
ispyb_server.serve_forever()
```



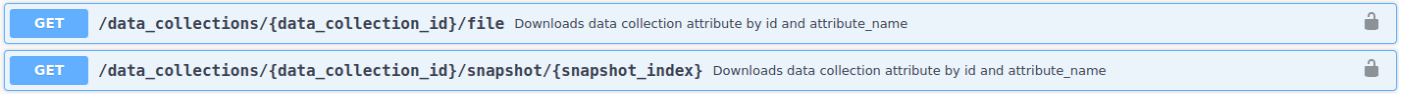
Documentation

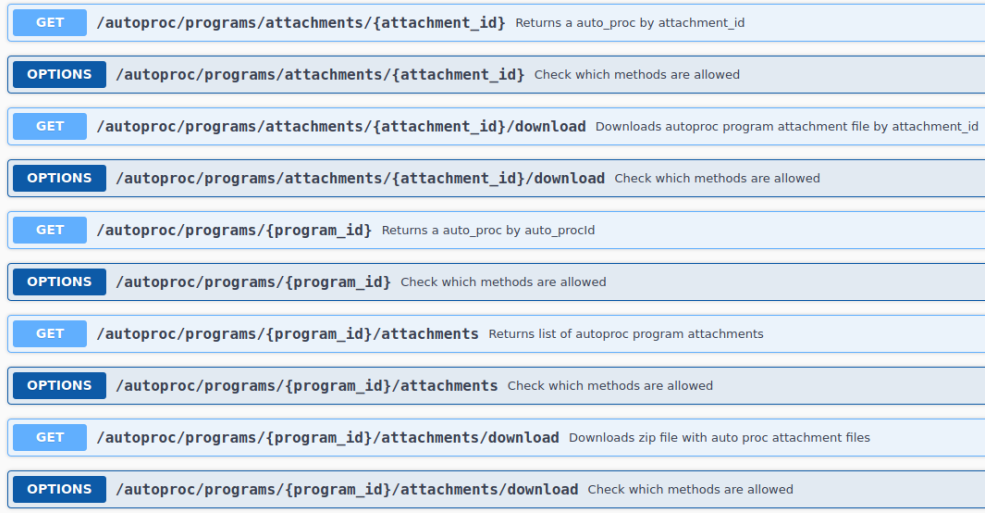
- Swagger ui to document and test api.



File download

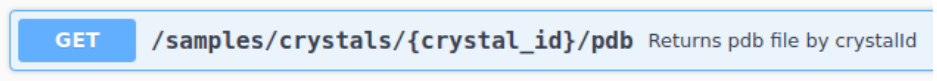
- Download autoproc program attachment files (single file by id and all files as a directory zip file).
- Download data collection snapshots and other associated files (image quality plot, Wilson plot).





Pdb files

- Upload/download pdb file. Link with https://www.rcsb.org/



- Downloads *.pdb if the file is on the filesystem. Preferred solution for manually edited pdb files.
- If pdb file is not available then download it from rcsb.org.

Dewar labels

- Dewar pdf labels are generated based on a html template.
- No pdf file templates, data fields etc. Avoids complicated pdf file handling.
- Template is filled based on pyispyb configuration and shipping info.
- Html file is converted to pdf with pdfkit.
- python-barcode and qrcode are used to generate barcode and qrcode.
- New directory static to store html template, images and other resources.

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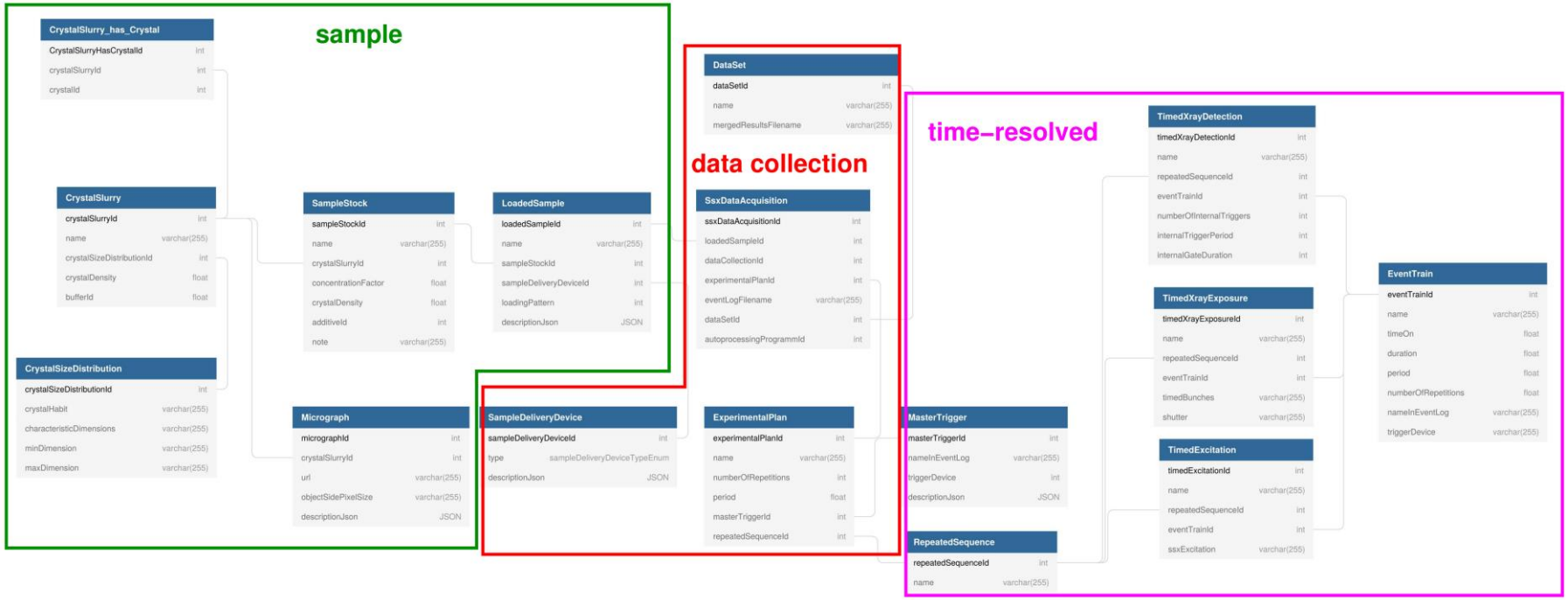
SSX data model



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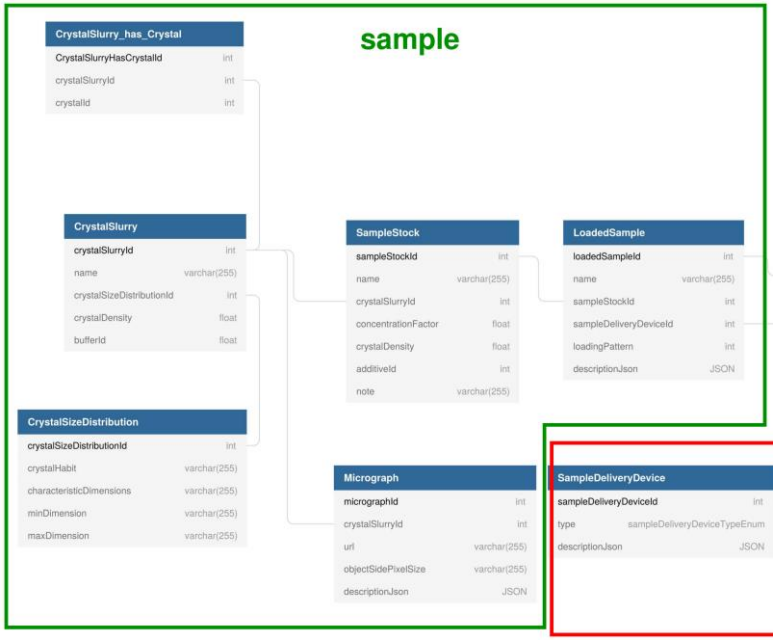
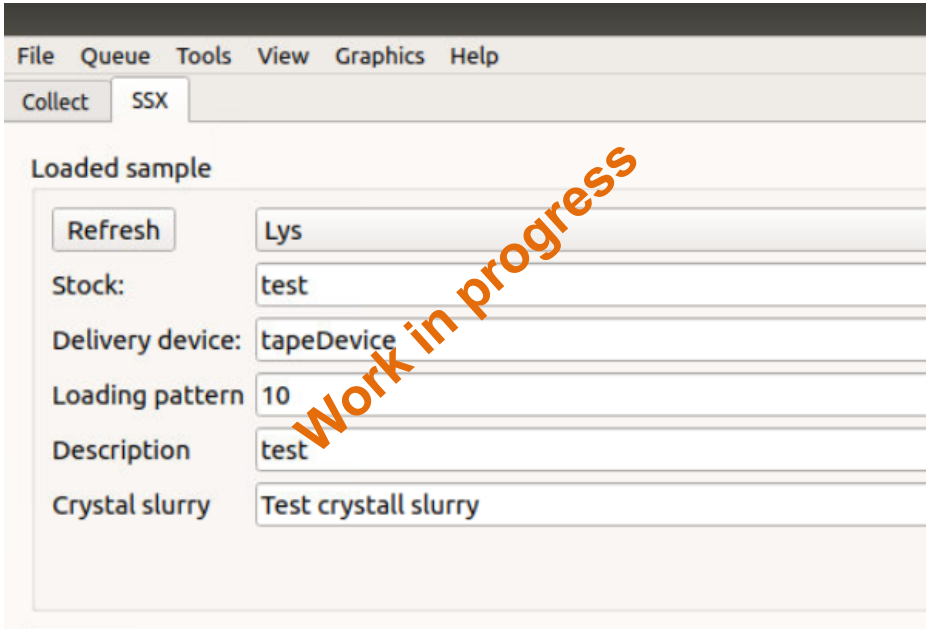
pyisypb and ssx

- Two new hardware objects for mxcubecore to access pyispyb REST API:
  - PyIspybClient.py
  - SsxIspybClient.py
- Prototype widget for mxcubeqt to acquire and store information about ssx samples.





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Thank you for your attention!