

Tools

- ▶ Fully automatic calculation system of electronic structure by First-principles
- ▶ nap (Nagoya Atomistic-simulation Package)
- ▶ Compound Prediction App
- ▶ Specific Heat Prediction App
- ▶ API Tools

LINK

- ▶ MateriApps
- ▶ Toki no Mori Wiki - Machine learning (Japanese only)

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API Tools

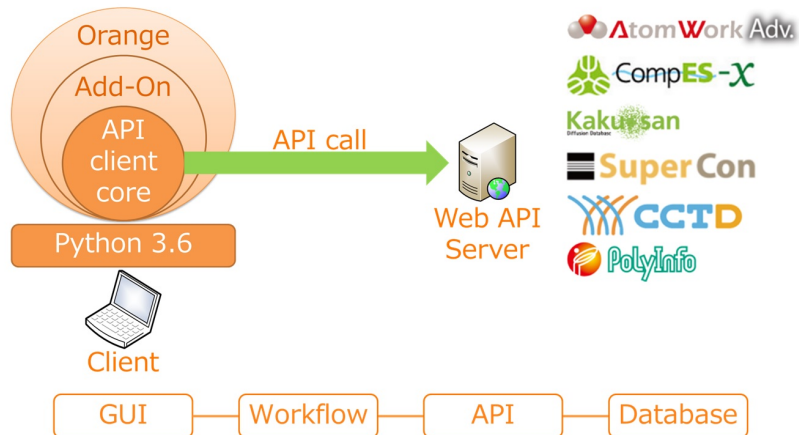
Overview

- Tools and environments to help you use the database API (Web API).
- You can use the following in the terminal room:

MatNavi by Orange	Data mining tool that can perform intuitive operation of Web API.
Jupyter Cloud	Python coding environment available from web browser.

MatNavi by Orange

"MatNavi by Orange" is a collaborated tool of "MatNavi ", the NIMS Material Database and "Orange", an open-source data-mining toolkit developed by University of Ljubljana.



At the first stage of providing DPF services, users were expected to have skills of Linux systems and (text-based) programming. The users also needed to learn data structures of WebAPI precisely.

Visual programming of "MatNavi by Orange" leads to easy learning of WebAPI and after mastering API, the users could step in machine learning by Python and automated First-principles calculation system as they understand deeper.

Jupyter Cloud

"Jupyter Cloud" is a Python coding environment that can be used from a Web browser without needing to construct an environment.

If you have "DPF Account", you can start using accessing from PC in the terminal room.

Libraries such as TensorFlow and pymatgen is installed. "WebAPI for MatNavi" can also be used.

	Python2	Python3	Python3.6 for RDKit
NumPy	1.16.2	1.16.2	1.15.0
pandas	0.24.2	0.24.2	0.22.0
Pymatgen	×	2019.3.27	2019.3.13
SciPy	1.2.1	1.2.1	1.2.1
Spglib	1.12.2.post0	1.12.2.post0	1.12.2.post0
COMBO	0.2	×	×
TensorFlow	1.13.1	1.13.1	1.6.0
Keras	2.2.4	2.2.4	×
scikit-learn	0.20.3	0.20.3	0.19.1
PyTorch	1.0.1.post2	1.0.1.post2	1.0.1.post2
RDKit	×	×	2017.09.1
DeepChem	×	×	2.1.0
mordred	×	×	1.1.1
XenonPy	×	×	0.3.2

 Only access from NIMS

Users can see "details of API Tools".