



AiiDA 1.0.0 Plugin Migration Guide

Sebastiaan Huber & Leopold Talirz

Steps

1. Decide new version & fix dependencies
2. Add python2/python3 compatibility
3. Fix imports using the `aiida-plugin-migrator`
4. Migrate calculations
5. Migrate parsers

Link to slides bit.ly/aiida-plugin-migration-guide

0. Install aiida-core develop branch

- `git clone`
https://github.com/aiidateam/aiida_core
- `cd aiida_core`
`git checkout develop`
- **Reusing existing clone?**
`find . -name "*.pyc" -delete`
- `pip install pip==18.1`
- `pip install -e .`
- `reentry scan`
- See docs on [installing rabbitmq](#)

`verdi status` # all services green?

1. Versioning

AiiDA uses *semantic versioning* - MAJOR.MINOR.PATCH

- Bug fixes => bump PATCH
- New Features => bump MINOR
- Backward-incompatible API changes => bump MAJOR

Suggestions for your plugin

- Any unreleased changes since your last release? => Make a new release
- Bump the MAJOR version for adding aiida-core 1.0 support and start with `alpha1` (so that people don't accidentally upgrade)
- Don't try to support aiida-core 0.12 and 1.0 in the same plugin version
- How to specify aiida-core dependencies:
 - `aiida < 1.0: aiida-core>=0.12.3,<1.0.0`
 - `aiida >= 1.0: aiida-core>=1.0.0b1,<2.0.0`

2. python2/python3

One way to do it: use a pre-commit hook

- add `.pre-commit-config.yaml` (see [here](#))
- add pre-commit extra in `setup.py` (see [here](#))
- `pip install -e .[pre-commit]`
- `pre-commit install`
- `pre-commit run --all-files`
(Only needed once)

3. aiida-plugin-migrator

aiida-plugin-migrator

- There's a long [list of backward-incompatible changes](#)
- plugin migrator reduces tedious search & replace
- It isn't perfect - PRs welcome!
- Getting "parsing failed" error?
Complete step 2 first.

3. aiida-plugin-migrator

Installation

The `aiida-plugin-migrator` only runs under `python3` (but it does *not* depend on `aiida-core`).

```
git clone https://github.com/aiidateam/aiida-plugin-migrator
cd aiida-plugin-migrator
pip install -e .

# need latest bowler fixes
pip install git+https://github.com/facebookincubator/Bowler.git@master
```

This adds `aiida-plugin-migrator.py` to the `PATH` .

Usage

```
aiida-plugin-migrator.py /path/to/plugin/code
```

4. Migrate Calculations

- see [instructions on the Wiki](#)

5. Migrate Parsers

- see [instructions on the Wiki](#)

6. setting up Travis-CI

- add `travis.yml` (see [here](#))
- register on `travis.ci.org`
- add github repo and enable tests

 aiida-zeopp



 Settings

The next commit to your repo will trigger the build.

plugin migrations in progress

- aiida-cp2k: [see PR](#)
- aiida-codtools
 - migration started in [provenance_redesign branch](#)
 - see e.g. [cif_base calculation](#)
- aiida-zeopp:
 - migration started in [release_v1.0.0a1 branch](#)

Acknowledgements

Supported by



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ERC
erc.europa.eu

Developers

The Materials Cloud And AiiDA teams



Marco
Borelli
(EPFL)



Sebastiaan
P. Huber
(EPFL)



Boris
Kozinsky
(BOSCH)



Snehal P.
Kumbhar
(EPFL)



Leonid
Kahle
(EPFL)



Nicola
Marzari
(EPFL)



Elsa
Passaro
(EPFL)



Giovanni
Pizzi
(EPFL)



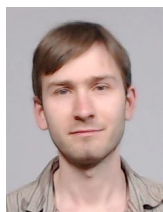
Thomas
Schulthess
(ETHZ,CSCS)



Berend
Smit
(EPFL)



Leopold
Talirz
(EPFL)



Martin
Uhrin
(EPFL)



Joost
VandeVondele
(ETHZ,CSCS)



Casper
Welzel
(EPFL)



Aliaksandr
Yakutovich
(EPFL)



Spyros
Zoupanos
(EPFL)

Contributors for the 23+ plugins: [Quantum ESPRESSO](#), [Wannier90](#), [CP2K](#), [FLEUR](#), [YAMBO](#), [SIESTA](#), [VASP](#), ...

Contributors to `aiida_core` and former AiiDA team members — Valentin Bersier, Jocelyn Boullier, Jens Broeder, Andrea Cepellotti, Fernando Gargiulo, Dominik Gresch, Rico Häuselmann, Eric Hontz, Christoph Koch, Espen Flage-Larsen, Andrius Merkys, Nicolas Mounet, Tiziano Müller, Riccardo Sabatini, Ole Schütt, Phillippe Schwaller

The CSCS support teams

Contacts and info



Website: aiida.net

Docs: aiida-core.readthedocs.io

Git repo: github.com/aiidateam/aiida_core/

Plugin registry: aiidateam.github.io/aiida-registry



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Materials Cloud: materialscloud.org

- **Archive:** archive.materialscloud.org
- **AiiDA Lab:** aiidalab.materialscloud.org
- **Quantum Mobile:** materialscloud.org/work/quantum-mobile

3 open positions for research software engineers/materials scientists
nccr-marvel.ch

Conclusions



- Workflows & Daemon help with automation
- AiiDA graph = map of the data jungle
- Your calculations are ready for Open Science
- FAIR sharing of data
- Free: 5 GB/record (50 GB for AiiDA graphs)
- write simple apps in python
- Run where you like:
 - on your machine (your machine, your setup)
 - on Quantum Mobile (your machine, our setup)
 - on AiiDA Lab (our machine, our setup)

