

## Domain-specific examples for atom probe tomography and field ion microscopy

!!! warning "Attention"

We are currently working to update this content.

Build upon your understanding of NOMAD's features with domain-specific examples and explanations.

### Contextualization for the technique and the scientific domain

A variety of file formats are used in the research field of atom probe tomography (<https://www.nature.com/articles/s43586-021-00047-w>) to document atom probe measurements and computer simulations. The pynxtools-apm plugin of the pynxtools parsing library solves the challenge of how these formats can be parsed and normalized into a common representation that increases interoperability and adds semantic expressiveness.

- pynxtools-apm (<https://fairmat-nfdi.github.io/pynxtools-apm/>)

The plugin uses the ifes\_apt\_tc\_data\_modeling Python library ([https://github.com/atomprobe-tc/ifes\\_apt\\_tc\\_data\\_modeling](https://github.com/atomprobe-tc/ifes_apt_tc_data_modeling)) that is developed together with the International Field Emission Society (<https://fieldemission.org/>).

### Work with standardized atom probe data in NOMAD and NORTH

Once standardized, NXapm-compliant data in NOMAD can be explored with domain-specific software tools using a convenient JupyterHub-based service offered by the NOMAD Remote Tools Hub (NORTH).

For this you should go to `Analyze` (menu bar) and select `NOMAD Remote Tools Hub`. If you are using the public Oasis the hub is available here (<https://nomad-lab.eu/prod/v1/gui/analyze/north>). This service and toolset of NOMAD offers a set of preconfigured containers. We have configured the `apmtools` container to provide you an example

of the capabilities that come with such customizable containers interfaced to an Oasis.

Mind that if you are using a local Oasis the hub may not have been activated and that specific containers need to be pull from the container registry as they are not part of a default Oasis development installation.

Currently, ``apmtools`` is a specific docker container that offers a graphical user interface

through the web browser that serves your NOMAD GUI. The container includes three data analysis tools:

- aptyzer (<https://github.com/areichm/APTyzer>) by Alexander Reichmann et al.
- paraprobe-toolbox (<https://gitlab.com/paraprobe/paraprobe-toolbox>) by Markus Kühbach et al.
- apav (<https://gitlab.com/jesseds/apav>) by Jesse Smith et al.

The container is configured such that the data in your uploads are available via the ``/config/uploads`` sub-directory from within the container. Thereby, you can move data in between the container. The connection between the container image and NOMAD allows

you to enrich your upload with specific post-processing results generated by any of the tools in the container.

The paraprobe-toolbox exemplifies how NeXus can be used to document the specific settings

and results of such processing via an open standard and documentation.

The ``apmtools`` container comes with a collection of getting started tutorials via a ``Cheatsheet`` jupyter notebook which you can access from the ``/home/atom_probe_tools``

sub-directory. Details dependent on the specific configuration of your NOMAD OASIS.