

Pychron: Automated Data Collection and Reduction for Noble Gas Geochemistry and Ar/Ar Geochronology

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Software

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Summary

Software is an essential part of the extraction, measurement, data collection, and data processing of noble gases from geologic samples. Noble gas laboratories use highly customized ultra-high vacuum systems and mass spectrometers for extracting and measuring the isotopic composition of geologic samples. Pychron was originally developed for Ar-Ar geochronology, where the ratios of five isotopes of argon are measured to precisely calculate the geologic age or thermal history of the sample.

Statement of need

The proliferation of inexpensive computing hardware and open source software has greatly benefited noble gas geochemistry, allowing for the full automation of the extraction and measurement process. Storage of raw isotopic measurements and metadata in central relational database management systems (RDBMS) such as MySQL have dramatically increased the quality and throughput of analytical data from Ar-Ar facilities.

Although software has long been recognized as a critical element of noble gas laboratory infrastructure, little community collaboration currently exists to develop and maintain robust, functional and sustainable software. Many laboratories either lack the full functionality they desire or have unsustainable custom solutions.

Description

Starting in 2008, Pychron has been under developed at New Mexico Geochronology Research Laboratory, forming the basis for a sustainable software ecosystem for noble gas geochemistry. Pychron is a fully featured, open source, python-based application used for data acquisition and processing in noble gas geochemistry and is now being used at a growing number of laboratories around the world. Written in python, Pychron uses many standard and third party libraries such as numpy ([Harris et al., 2020](#)), scipy ([Virtanen et al., 2020](#)), uncertainties ([Lebigot, 2010](#)) for computational aspects and Enthought Tool Suite/Qt for a rich customizable UI.

Pychron supports single and multi-collector automated real-time data collection with mass spectrometers from Thermo Scientific, Isotopx and Pfeiffer and is readily adapted to other instruments. Legacy data collected using older MAP and Nu instruments is accessible via Pychron. Pychron uses an extensible plugin architecture making it highly configurable and adaptable to various hardware setups.

The data reduction process is based on a “pipeline” model offering a flexible and configurable workflow for bulk processing data. Pychron uses a custom data management model called “Data Version Control,” that combines a Git-based file versioning system with a relational database.

We have always envisioned Pychron as a community-based development project and welcome contributions and encourage users to provide feedback, bug reports and feature requests, via GitHub’s issue system at <https://github.com/NMGRL/pychron>.

Active Laboratories

Pychron is used at a growing number of noble gas laboratories throughout North America.

- New Mexico Geochronology Research Laboratory, New Mexico Bureau of Geology
- University of Manitoba
- WiscAR, University of Wisconsin
- SWIRL, US Geological Survey - Denver
- AGES, Lamont-Doherty Earth Observatory, AGES
- US Geological Survey - Menlo Park
- MNGRL, NASA-Goddard Space Flight Center
- AEL-AMS, Ottawa
- ANGL, University of Arizona
- TAP, Purdue University
- HAL, University of Indiana Urbana-Champaign
- University of Florida

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