

DATA ECOSYSTEM

Facts and figures 2019-2020

MaX offers a materials ecosystem for automated high-throughput calculations and automatic storage of data in graph databases.

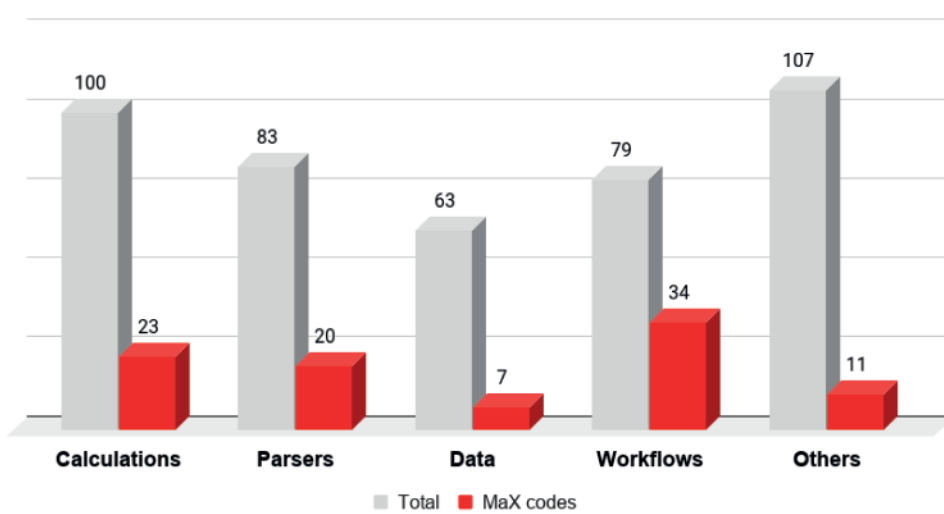
AiiDA



as the working environment.

- 52 registered plugin packages
- ~ 80 workflows
- 32% of calculations and workflows plugins supported directly by MaX

Plugins registry and use



AiiDA simplifies the task of sharing the results thanks to its coupling with the Materials Cloud, where data can be uploaded, visualized, analyzed and shared.

MATERIALS CLOUD



MATERIALSCLOUD

as the cloud simulation and the web dissemination and sharing platform.

9'978'441

crystal structures

7'502'686

structures with associated DFT SCF calculations

2'455'694

data and calculation nodes

321'970

reproducible calculations

Research data management and stewardship is streamlined providing an integrated platform for FAIR data sharing:

Materials Cloud is an implementation network of GO FAIR. It also acts as a simulation platform, providing tools to enable running new simulations both on premises and in the cloud via



also registered as a service on the European Open Science Cloud (EOSC)



a virtual machine for computational materials science

and a number of online interactive tools.