MAX
DRIVING THE EXASCALE TRANSITION

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.
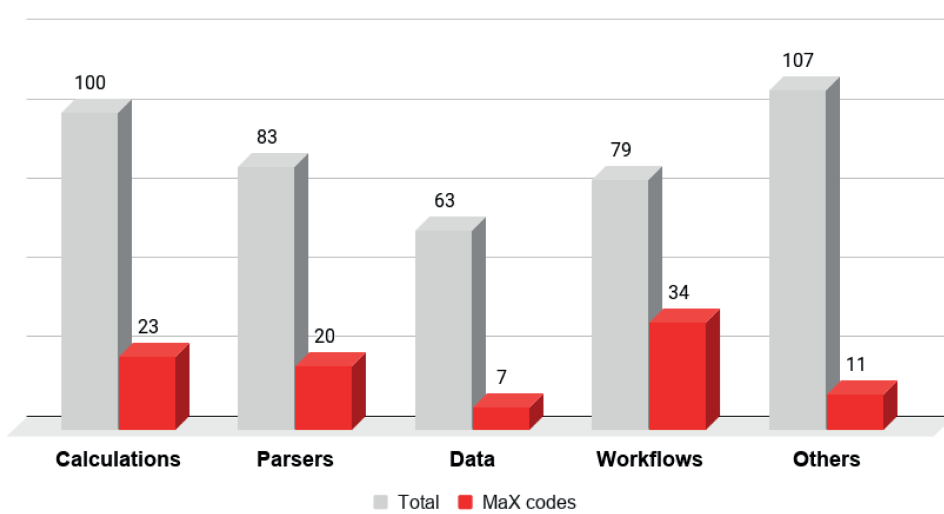
AiiDA

as the working environment.

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

Plugins registry and use

	Calculations	Parsers	Data	Workflows	Others
Total	100	83	63	79	107
MaX codes	23	20	7	34	11

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

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

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

QUANTUM MOBILE
a virtual machine for computational materials science

and a number of online interactive tools.

31 MAY 2020