MAX DRIVING THE EXASCALE TRANSITION
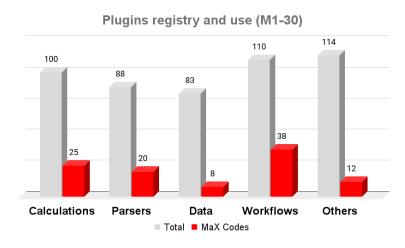
DATA ECOSYSTEM
Facts and figures 2020-2021

MAX offers a materials design ecosystem for running high-throughput calculations with automated data storage in graph databases.

AiiDA

AiiDA

as the workflow engine

» 61 registered plugin packages
» ~110 workflows
» 21% of calculations and workflows plugins supported directly by MAX

Plugins registry and use (M1-30)

	Calculations	Parsers	Data	Workflows	Others
Total	100	88	83	110	114
MaX Codes	25	20	8	38	12

■ Total ■ MaX Codes

Results obtained with AiiDA workflows can be easily shared thanks to its close integration with the Materials Cloud, where data can be uploaded, visualized and analyzed.

www.aiida.net

MATERIALS CLOUD

MATERIALSCLOUD

as the web dissemination platform

Materials Cloud is recommended as a data repository for Materials Science by Nature's *Scientific Data* and by the EU Commission's *Open Research Europe* journals

www.materialscloud.org

22'145 443
crystal structures

7'521'504
structures with associated
DFT SCF calculations

2'965'252
data and calculation nodes with
full AiiDA provenance

674'778
reproducible calculations
with full AiiDA provenance

AiiDALAB

AiiDAlab

as the cloud simulation environment

AiiDAlab provides the user with a dedicated and intuitive simulation environment directly in the cloud or on remote or local resources.
Here the user can run and manage AiiDA workflows with tailored lightweight web applications, all from the browser.

www.materiarscloud.org/work/aiidalab

31 MAY 2021