



NOVEL MATERIALS DISCOVERY

Title

WP1

PI Meeting, 6. Feb 2018, London

Fawzi Mohamed FHI Berlin



NOMAD

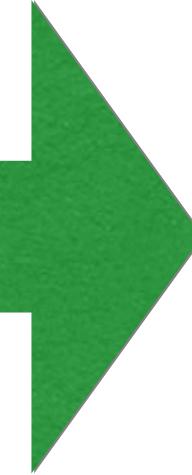
NOVEL MATERIALS DISCOVERY

NOMAD
REPOSITORY

NOMAD Archive: Goal

NOMAD Archive

Make data of the simulation codes
used in the community accessible



WP2: NOMAD
ENCYCLOPEDIA

WP3: NOMAD
VISUALIZATION

WP4: BIG DATA
ANALYSIS

External users



NOVEL MATERIALS DISCOVERY

NOMAD Archive: What is it

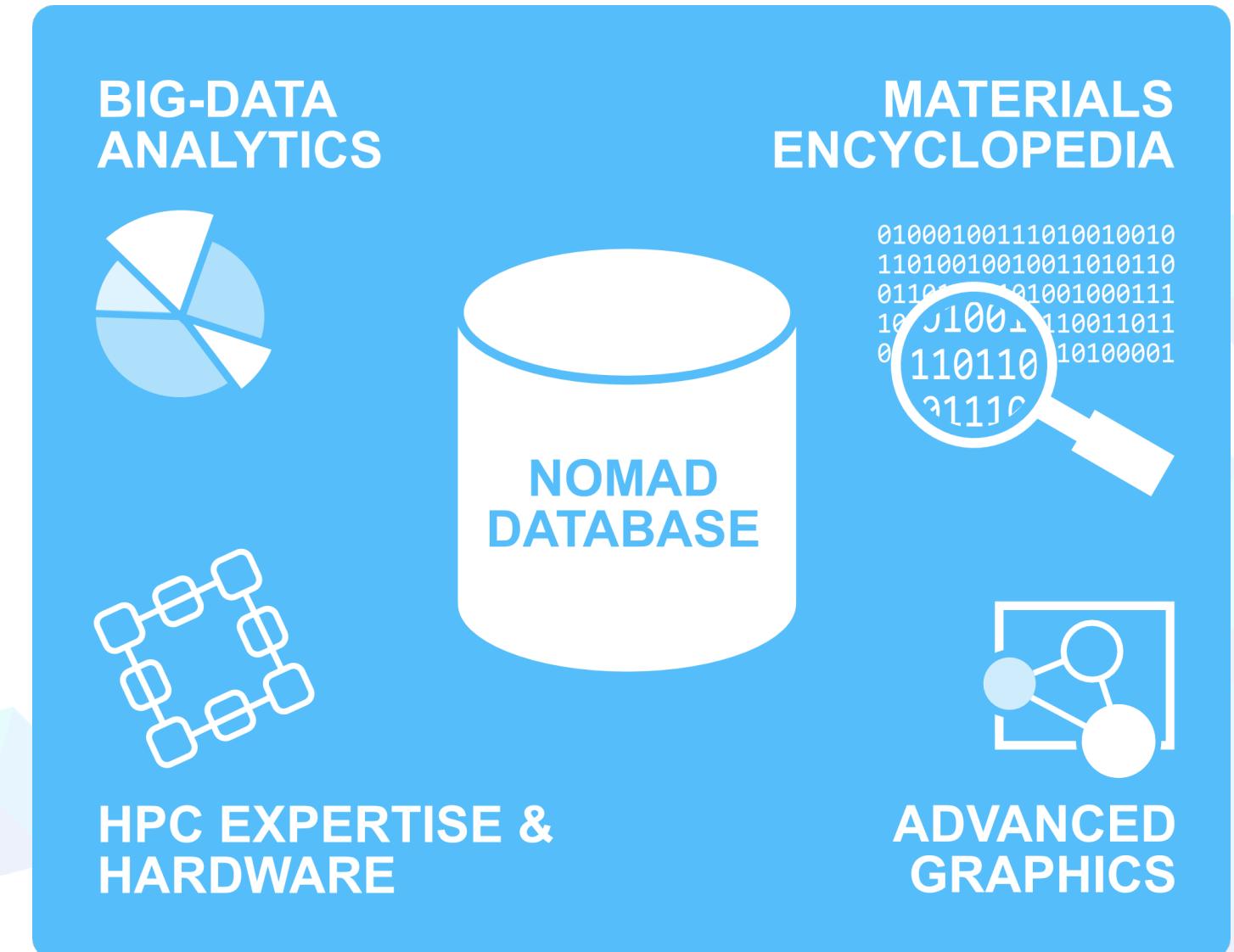




NOVEL MATERIALS DISCOVERY

The core of the
NOMAD Database

NOMAD Archive: What is it





NOVEL MATERIALS DISCOVERY

Work Done

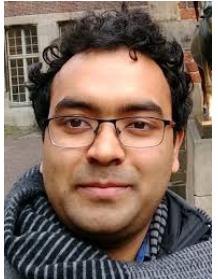
- Repository integration
- Documentation
- First version of the resolve & query API
- Parsers (ongoing)



NOVEL MATERIALS DISCOVERY

Who

- Low level infrastructure
- Higher level infrastructure
- Documentation
- Repository
- Parser development



(Ankit Kariyaa)
FHI



(Alfonso Sastre)
FHI



Fawzi Mohamed
FHI



Berk Onat
Warwick



(Yazid Hamdi)
FHI



Jungho Shin
HUB



Nicolas Fabas
MPCDF



Arvid Ihrig
FHI



Thomas Zastrow
MPCDF



Archive & Parser Developers

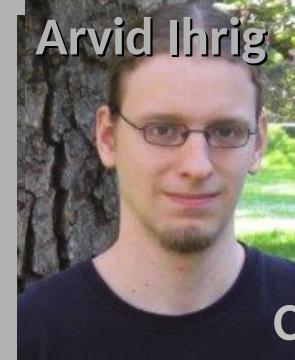
(Ankit Kariyaa)



(Alfonso Sastre)



Arvid Ihrig

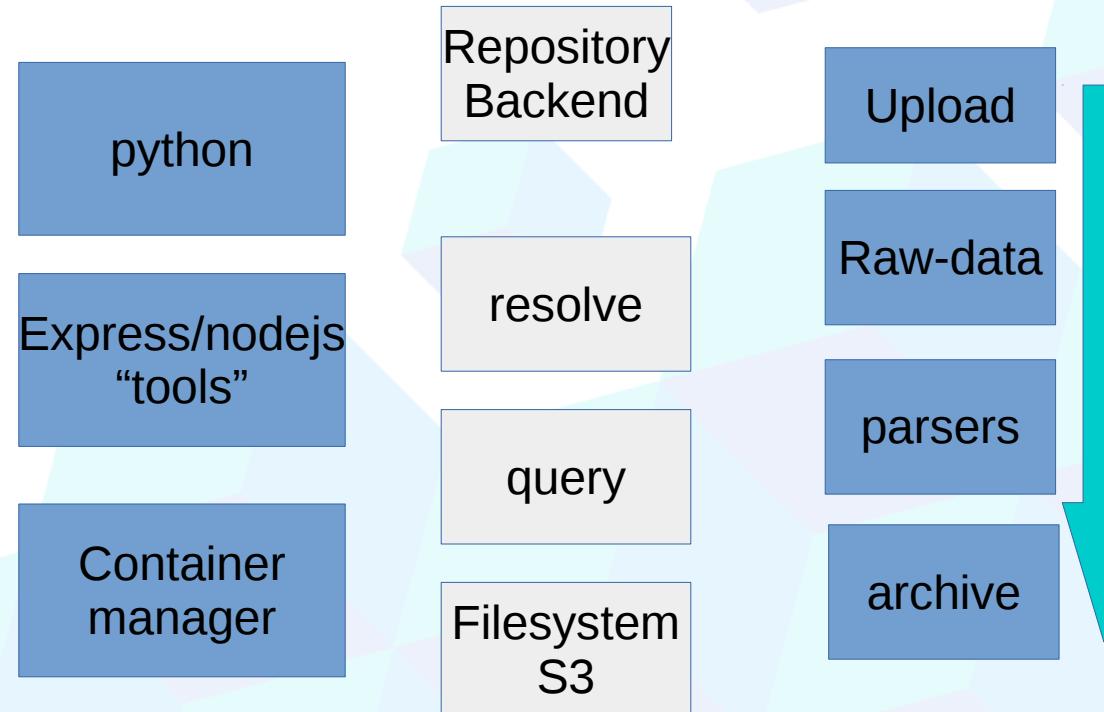




NOVEL MATERIALS DISCOVERY

Where we want ot go

- Robust infrastructure
- Simplified deployment for developers and mirrors
- Docker, Kubernetes (and helm)
- Metainfo
- Infrastructure for „tools“
 - Nodejs/express
 - Python encyclopedia
- Container-manager
 - Analytics, but not only





NOVEL MATERIALS DISCOVERY

Hackaton

- End of march
- Focus on Infrastructure
- Analytics tools, tools
- Mustafa & Abdul (new people) present