

NOMAD

THE NOMAD LABORATORY

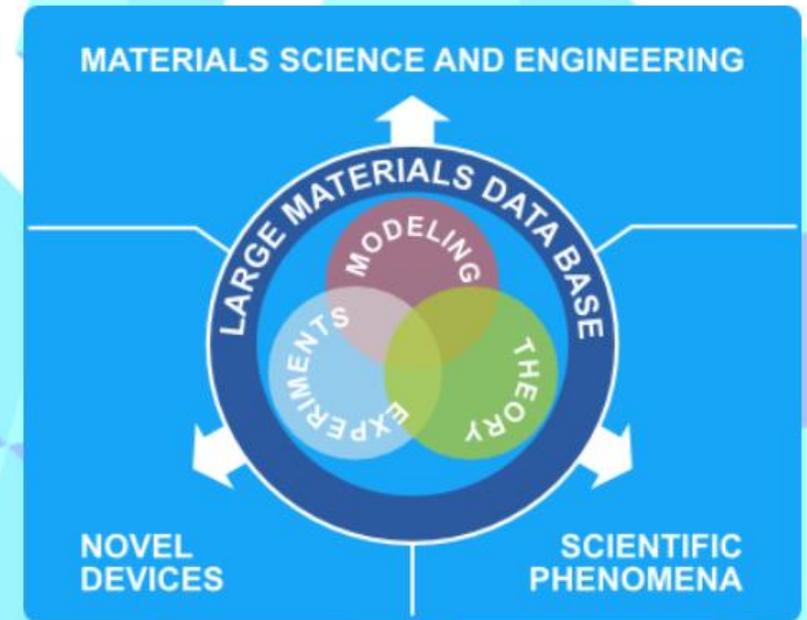
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The Novel Materials Discovery (NOMAD) Laboratory develops a Materials Encyclopedia and Big-Data Analytics tools for materials science and engineering.

Eight complementary computational materials science groups and four high-performance computer centers form the synergetic core of this Centre of Excellence.



MATERIALS ENCYCLOPEDIA



BIG-DATA ANALYTICS



ADVANCED GRAPHICS



HPC INFRASTRUCTURE



OUTREACH

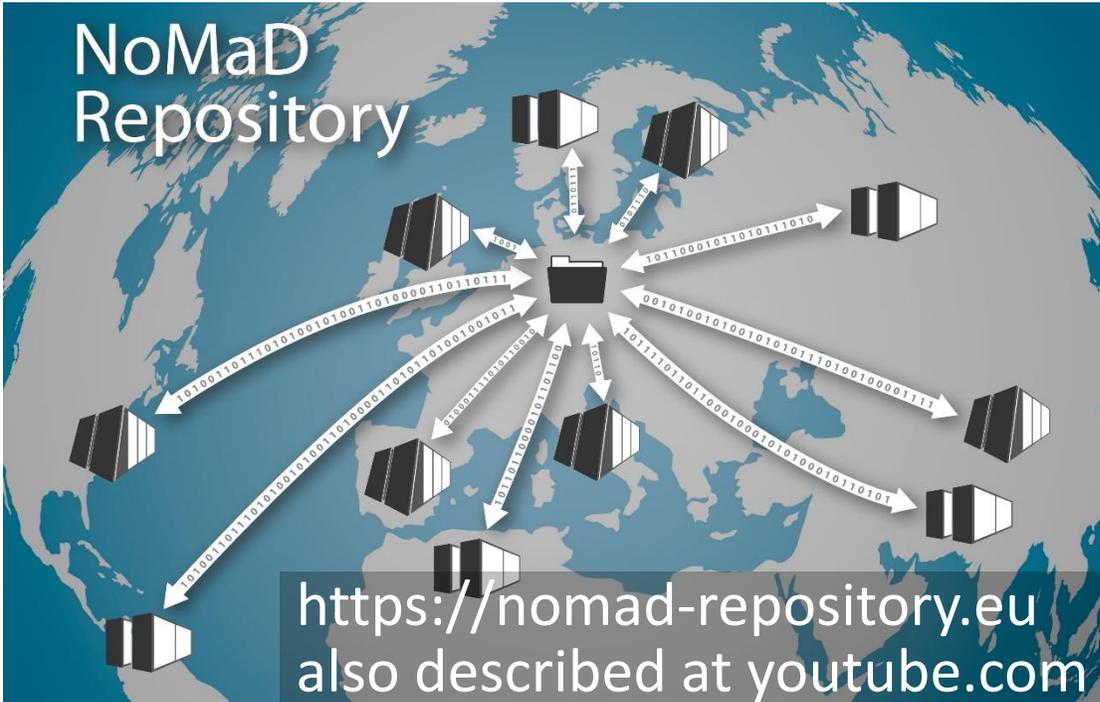


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NOVEL MATERIALS DISCOVERY

NoMaD
Repository



The NoMaD Repository accepts (and requests) in- and output files of all important codes. Currently, the NoMaD Repository contains **3,026,745** entries.

There are 30-40 important codes used in computational materials science.

Nomenclature, data representation, and file formats of the input and output files of these codes are different. The heterogeneity could hardly be worse.

<http://NOMAD-CoE.eu>

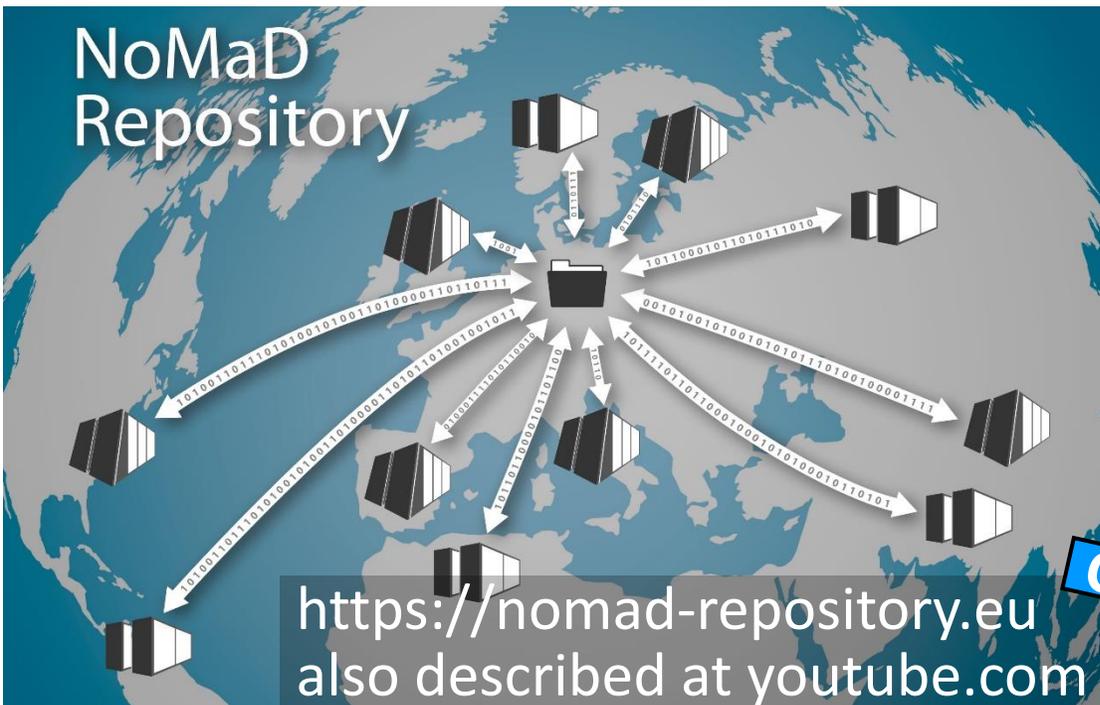


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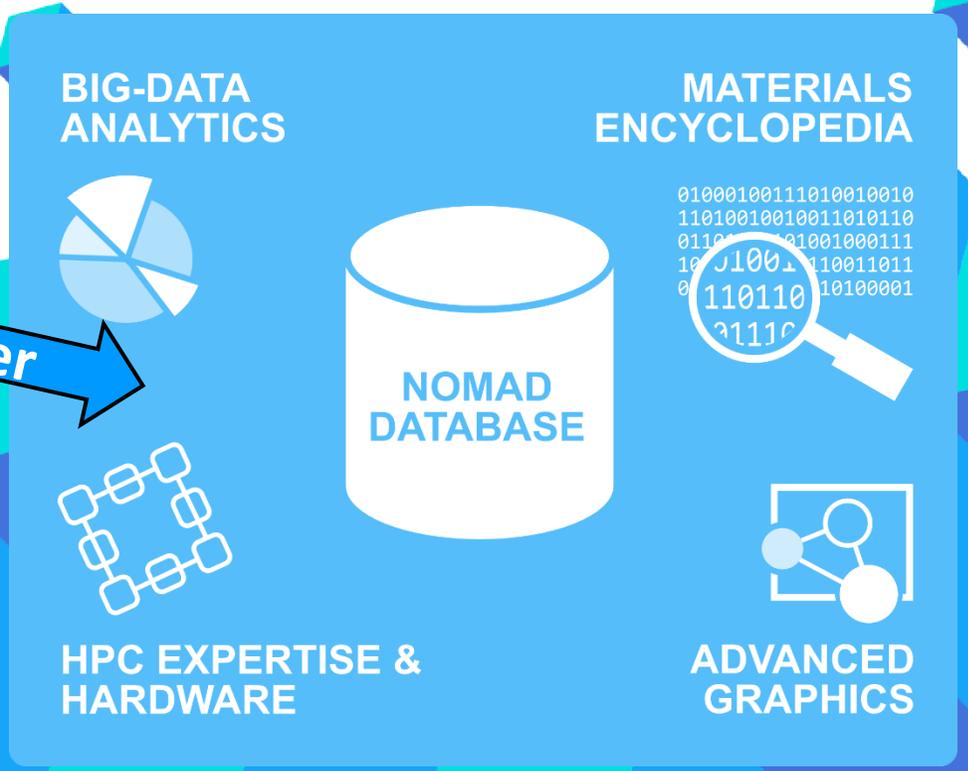
NoMaD Repository



The NoMaD Repository accepts (and requests) in- and output files of all important codes. Currently, the NoMaD Repository contains **3,026,745** entries.



Conversion Layer

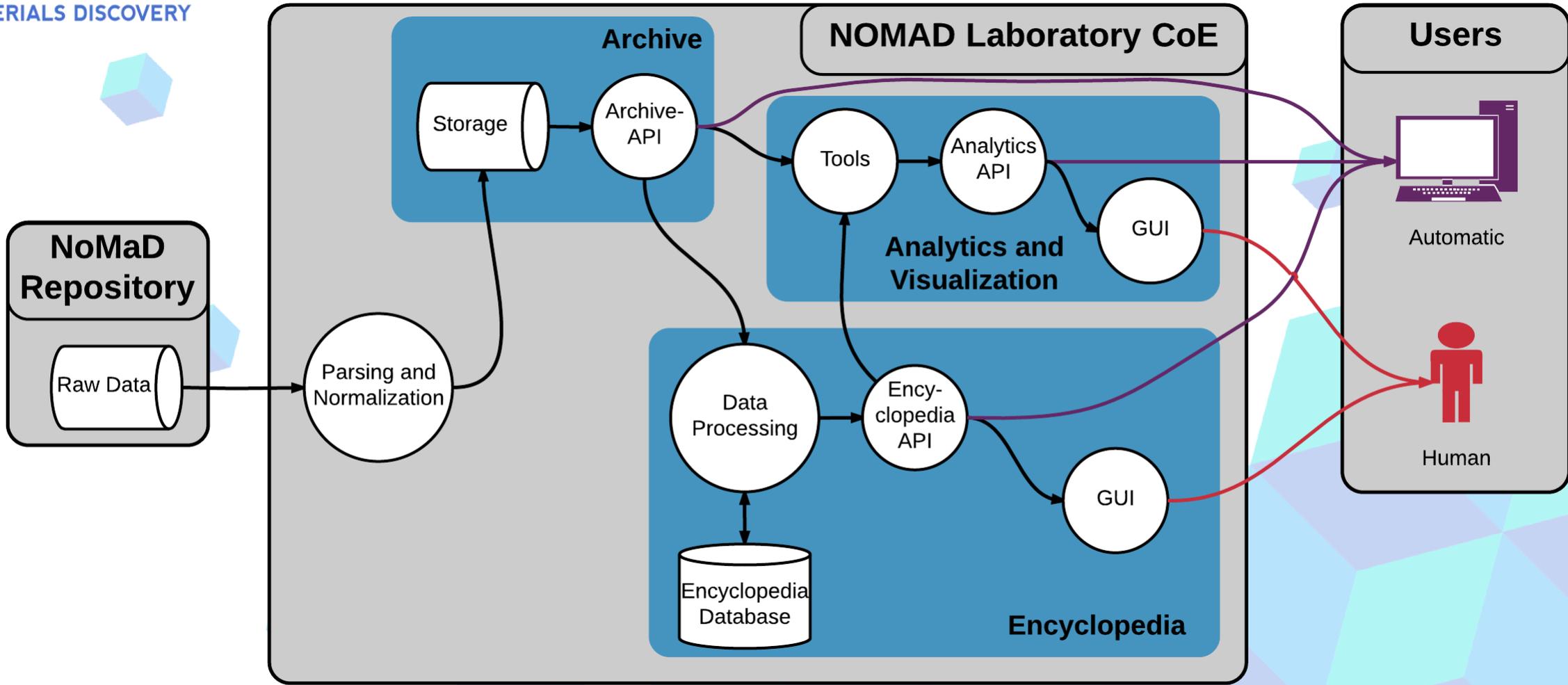


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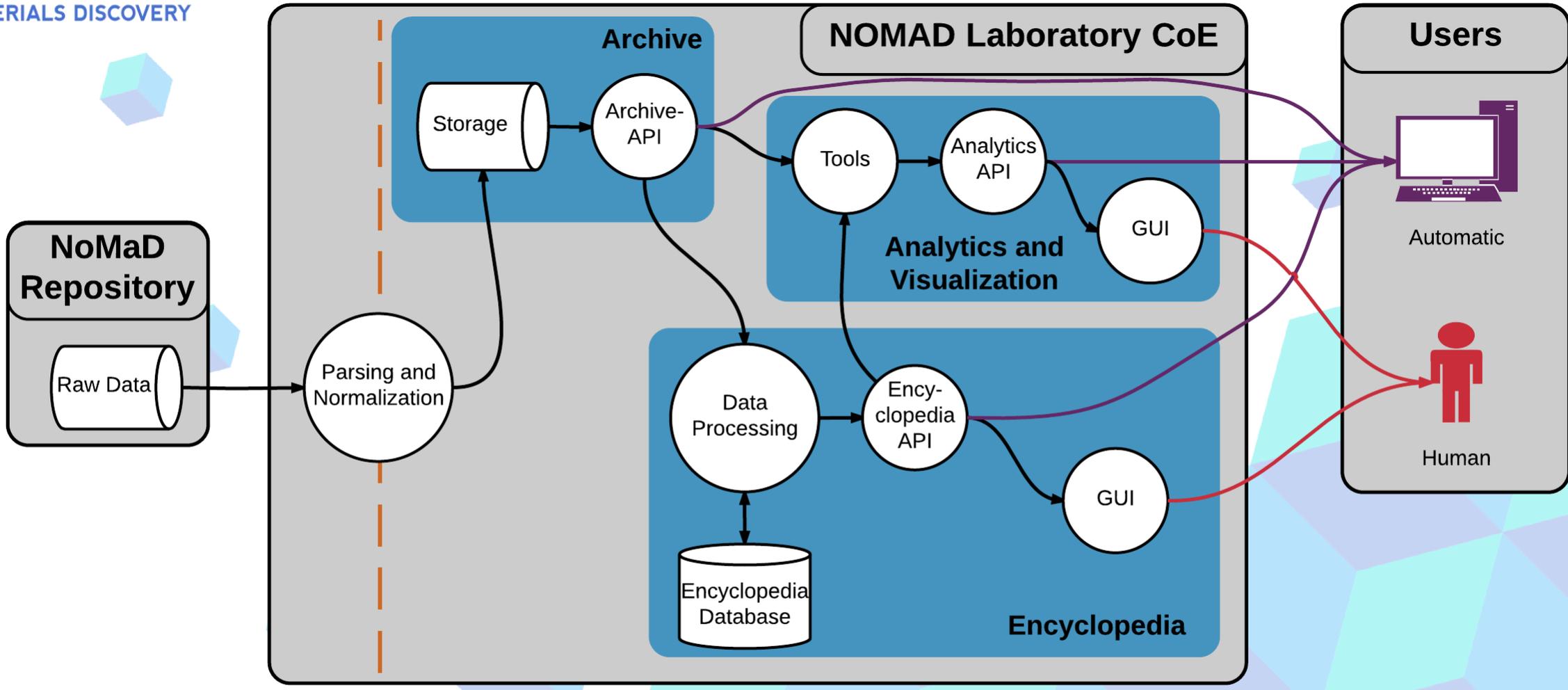
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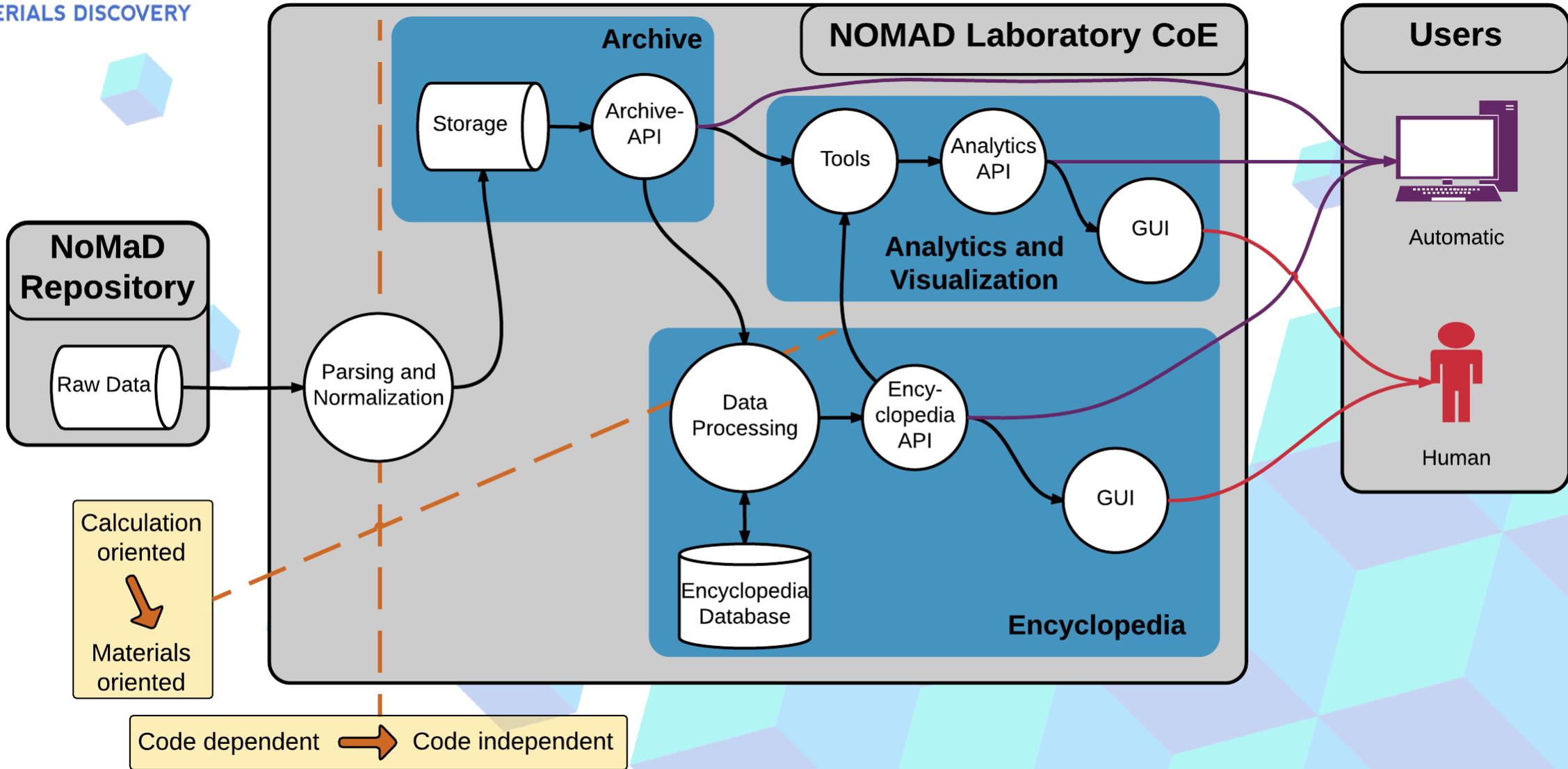


Code dependent → Code independent



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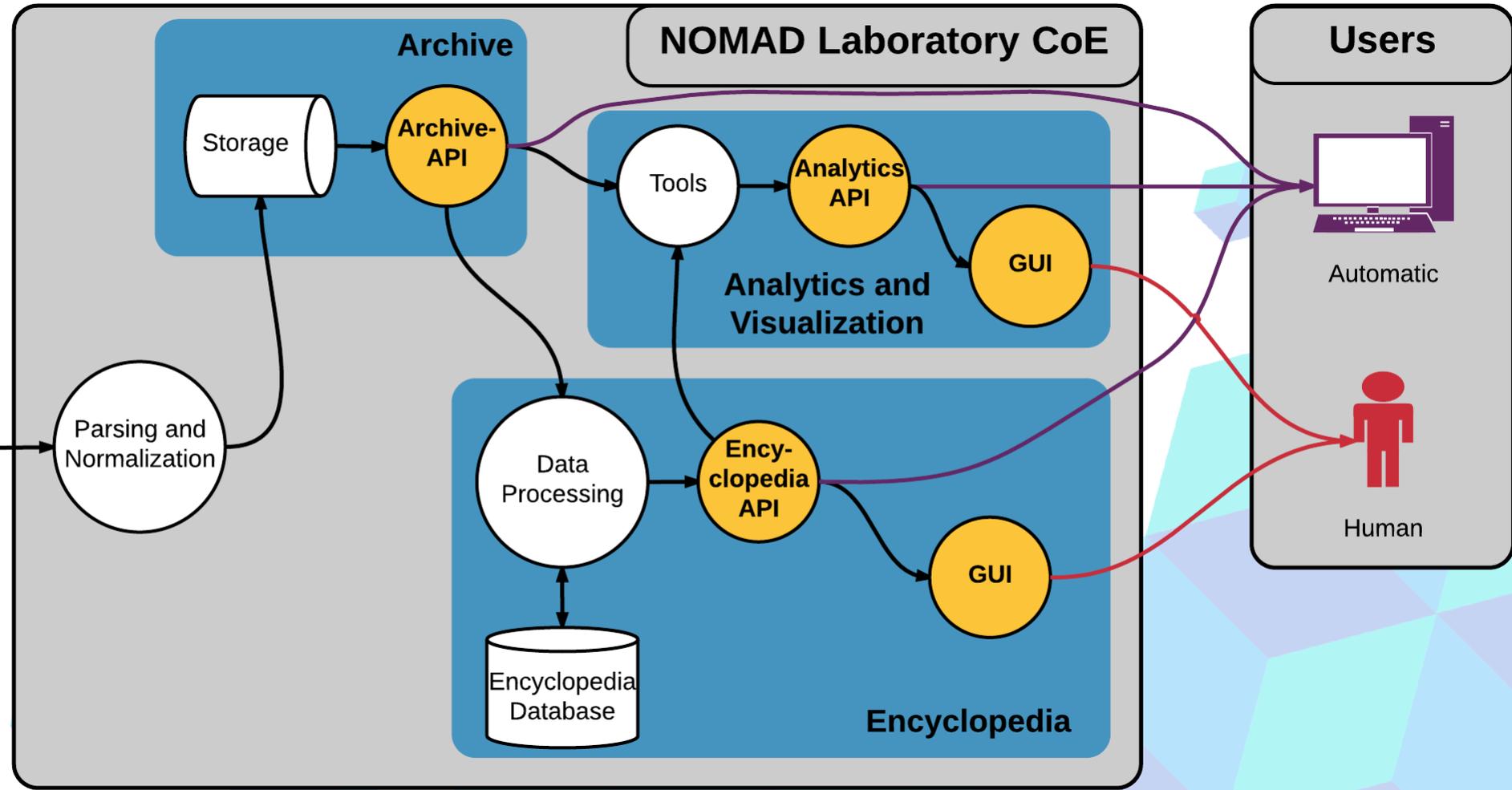
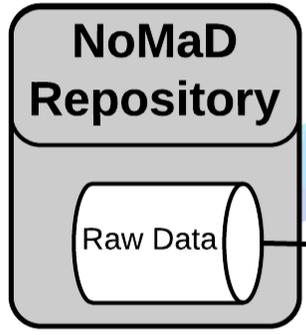


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Services (Ecosystem)





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Services



Main categories:

- Calculation and materials databases
- Materials encyclopedia
- Analytics tools
- Advanced graphics

Calculations on demand
(generating data missing for specific scientific challenges)

NOMAD tools for high throughput screenings highly valuable



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Meeting EU objectives

Tackling the question „What to do with all the data“

„Classic“
HPC

Distributed

- Storage
- Processing
- Services

Provides

- Verification and quality assurance for calculation data (also: „error bars“ project -> establishing trust levels)
- Data-oriented education



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Meeting EU objectives

- Developments also driven by user-input
 - Committees:
 - Scientific Advisory Committee (SAC)
 - Industry Advisory Committee (IAC)
 - ISVs are treated as industrial users and members of IAC (present at first industry meeting)
-
- IPR and Sustainability Plan (Deliverable 5.2, submitted)
 - Data Management Plan (Deliverable 8.2, submitted)

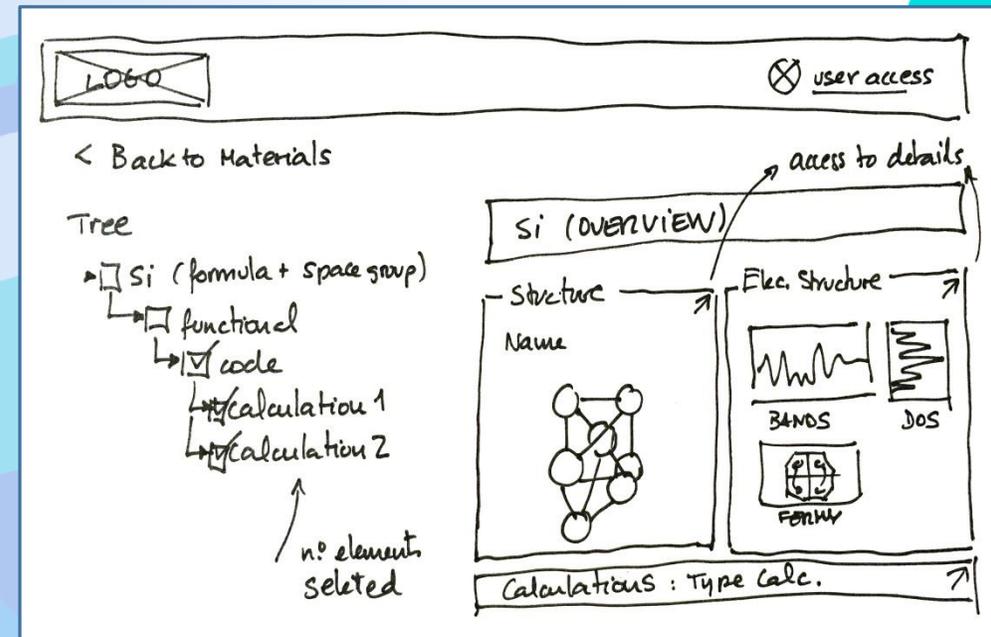
Questions Rome-meeting:

How to stimulate collaborations with other CoEs:
 Input for NOMAD:

Use-Cases (Encyclopedia)

- Basic input about expected functionality
- Influences prioritizing developments
- Can lead to scientific projects

Applies to any CoE with interest in materials (EoCoE, ...?)





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Questions Rome-meeting:

How to stimulate collaborations with other CoEs:

NOMAD can work with services of

- MaX: calculation services
 - Establishment of workflows
 - Setup of calculation environment
 - Execution of calculations
- POP: Analysis of performance-critical tools



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International cooperations:

Metadata for describing materials science calculations:

- Workshop in Lausanne about common standards
~20 codes present

Together with CECAM's ESCDF initiative for a common data format

- Discussions with NIST (USA)
- Contact with European Materials Modeling Council

Industry workshop (March 2016) interests (amongst others):

- Structure and stability of surfaces
- Catalyst screening for CO₂ activation
- Including Materials Encyclopedia in company-knowledge-base



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What can EXDCI do for int. cooperations:

Building awareness in industry about

- Data-oriented services of NOMAD
- What computational materials science can do

Helping with „creating a market“

- Dissemination, events

Finding synergies with FetHPC projects



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Relation with SRA:

- HPC (& DATA) usage models

- HPC (& DATA) services
- Education and training

- => bringing HPC and Big Data to the users!
(e.g. Materials Encyclopedia for „schoolkid“)

HPC in

- analytics
- and “hidden” in data



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Relation with PRACE:

Infrastructure needed for:

- Distributed services
 - Storage
 - APIs
 - Web-interfaces
 - Remote visualization

Using PRACE computing time for

- Large scale analytics
- Calculations

(e.g. as now prepared in Barcelona for CO₂ activation)

