NOMAD Archive

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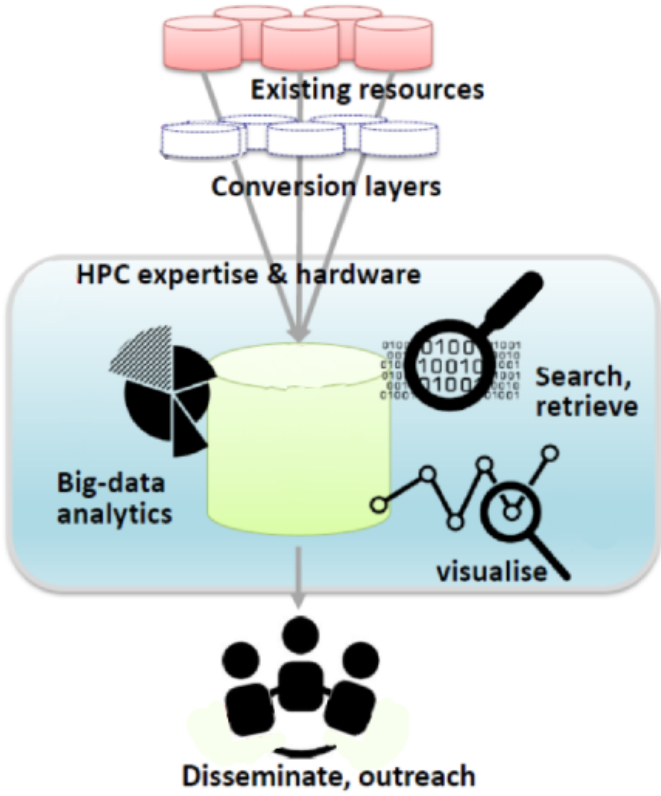
12.9.2016

NOMAD
NOVEL MATERIALS DISCOVERY

NOMAD Laboratory

- Start with open access calculations
- Data preparation (conversion layer)
- Big data analysis (insights)
- Visualization
- Materials Encyclopedia



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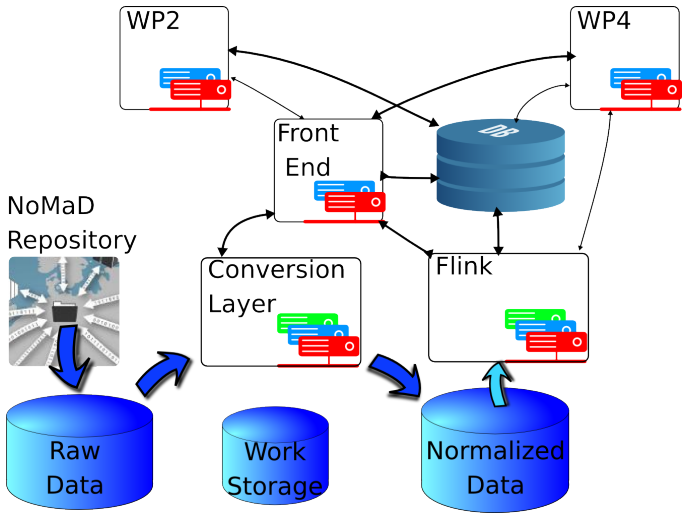
Conversion layer and NOMAD Archive

- data preparation step
- Start with public data from the NOMAD repository `http://nomad-repository.eu/`)
- start from many codes and go to a code independent representation
- enable big data analysis between and across different codes



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Big Data

- Big data in the data preparation phase is not primarily big amounts of data...
- ...but rather robust tools and work-flows.
- not just produce big amounts of data, but do so
- $\rightarrow$ in a reliable way
- $\rightarrow$ in a way that one can find problems, fix them
- ... and then integrate the correct data.

Naming and Provenance

- very important to achieve these goals
- about source of the data (a file,...)
- to describe the data itself

Description of a data source...

- public data from the repository `http://nomad-repository.eu/`
- create raw data archives using the BagIt format
- use a name depending only on their content (modification dates filename and content of the data)
- $\rightarrow$ archiveGid: "R" + a 28-character checksum
- storage independent uris: `nmd://<archiveGid>/path/in/archive`
- calculationGid: built from the uri of the main file of the calculation
- clear naming of the program used to transform the data: git describe for versions

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Description of the normalized files

- comes from archive X (raw data naming and nomad uri), and was produced parser Y version Z1
- So we can say: "replace (or compare) that data with the one using parser Y version Z2"

Description of the data

- we want to describe workflows and changes on the data itself
- We use metadata as our conceptual model of the data
- Metadata is the name or label that characterizes corresponding values. For example, “fcc lattice constant in nm” is a metadata and “0.526” may be the corresponding value. Thus, if one thinks of storing data as ‘key’–‘value’ pairs (as in a dictionary), the ‘key’ is the metadata.
- metadata is boring
- allow seamless extension

Meta data: our conceptual model

- define how the data that we extract is organized, and what it is
- important both for human and for the machine
- data values consist of simple data types and multidimensional arrays of them
- group together similar *types* making them inherit from the same type (all energies inherit from the *energy*)
- group together *values* with sections
- allow one to many relationships between sections (relational data model)

Metadata: available now

- common part: how to represent the common quantities found in calculations: energy, geometry, wavefunctions,...
- `https://nomad-dev.rz-berlin.mpg.de/ui/index.html`
-
- open git, you can contribute!

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Big data: speed and scalability

- Big Data is *also* about big amounts of data
- Optimization and being fast is important
- ability to scale, and use distributed resources

Parsers...

- extract information from simulation input and outputs to make it available for analysis
- information that is not extracted is invisible, a parser defines the data that can be analyzed
- to make the data processable in an automatic way it should be mapped to a clear model
- a parser is a mapping from the inputs and outputs of a calculation to data described by our metadata

Many codes...

- FHI-aims , VASP , turbomole , Dmol^3 , ORCA , TINKER , NAMD , exciting , WIEN2k , ELK , FLEUR , FPLO , Gaussian , GAMESS , NWChem , Molcas , GULP , onetep , CASTEP , LAMMPS , DL_POLY , LM Suite (TB-LMTO-ASA) , QUIP /libatoms/GAP , LAMMPS , cp2k , crystal , BigDFT , SIESTA , CPMD , Quantum Espresso , octopus , Smeagol , DFTB+ , abinit , GPAW , ASAP , gromacs , MOPAC
- ...many formats

Doing analysis with parsed result

- the goal of all this is doing the rest of NOMAD, so analysis
- obviously after so much preparation things...
- ... failed ...
- well not really but some things were wrong, or missing
- I imagine you know how we went to fix them
- not working around them, but fixing them and improving their detection and correction
- big data means doing similar thing many times, so we will encounter these problem again, and it should be easier to get rid of them

Inspect and Debug

- some parsers did not end $\rightarrow$ now the parse executer can be queried about what it is doing, and when it started
- we collect detailed statistics on the parsing and create a DD that can be queried to compare different parsers, find regressions,...
- we have automatic tests (and we will need many more)
- we want to make all these tools available to who does the analysis
- normally he know what he will want to check

Big Data Analysis

- testing an working on a parser is already big data analysis
- we try to already use some of the techniques for Big data analysis already here
- exploring notebooks
- support the parser developer, he knows best how to test

Generating calculations

- computer get faster
- it is easier to analyze output if you control the generation, you can have simpler analysis
- you can know things implicitly: calculation A and B be use compatible settings, because I generated like that
- NOMAD choose the more difficult path of try to help even analyzing calculations done by somebody else
- much more difficult, but
- produces more robust parsers
- everybody needs parsers, and gains from more robust parsers
- even if the idea of analyzing random inputs should fail