NOMAD Laboratory: the challenges of the conversion to a code independent representation

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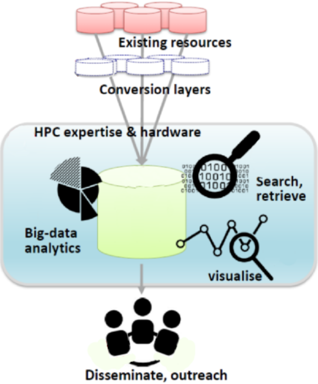
NOMAD CoE http://nomad-coe.eu/

- EU project started on the 1. Nov 2015
- 8 research centers
- 4 super computing centers
- 20 positions for highly qualified PhD students and postdocs

NOMAD Laboratory

- Start with calculations (public data from the repository `http://nomad-repository.eu/`)
- Data preparation (conversion layer)
- Big data analysis (insights)
- Visualization
- Materials Encyclopedia



Visualization

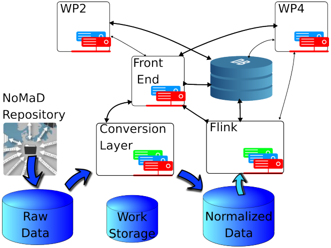
- Web based and VR (+ legacy
- Visualization of (periodic) systems, and densities
- visualization for data analysis

Big data analysis

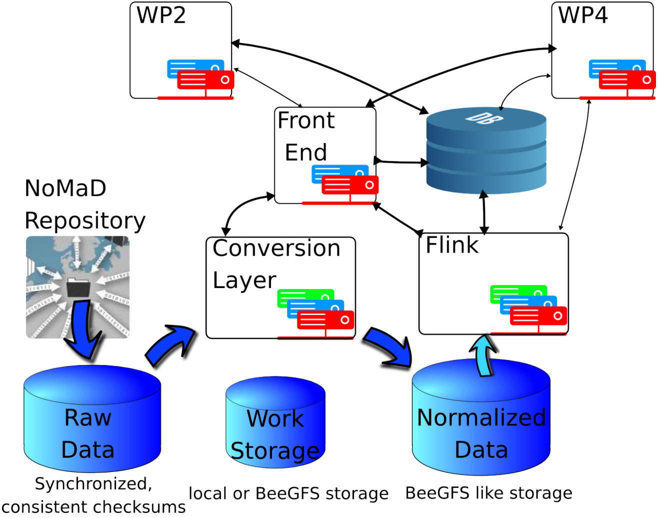
- Define new descriptors
- Discover trends
- Classification
- Create a toolbox to perform various kinds of analysis

NOMAD DB

- code independent representation
- Flink for map/reduce and more advanced queries
- enable big data analysis between and across different codes



High-level architecture



Map & reduce

- way to express some algorithms that makes them easy to parallelize, became popular after Google article
- can work well on distributed data

Flink

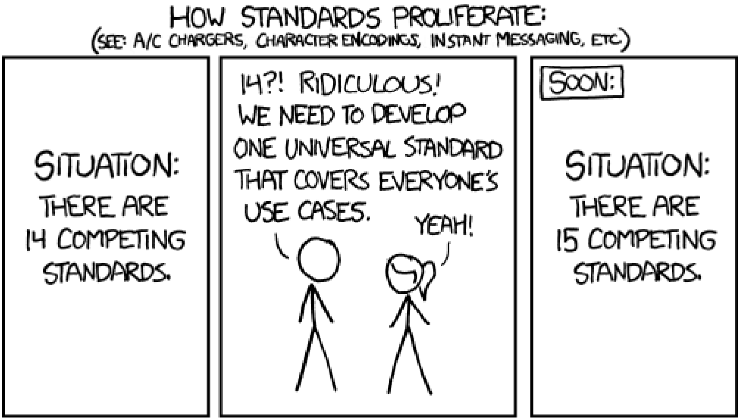
- Flink, started in Berlin
- One of the leading frameworks for data-flow and streaming optimization that improves on the map reduce approach
- Tries to support not just data-flow or stream processing but also iterative methods, graph processing and some machine learning algorithms

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

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

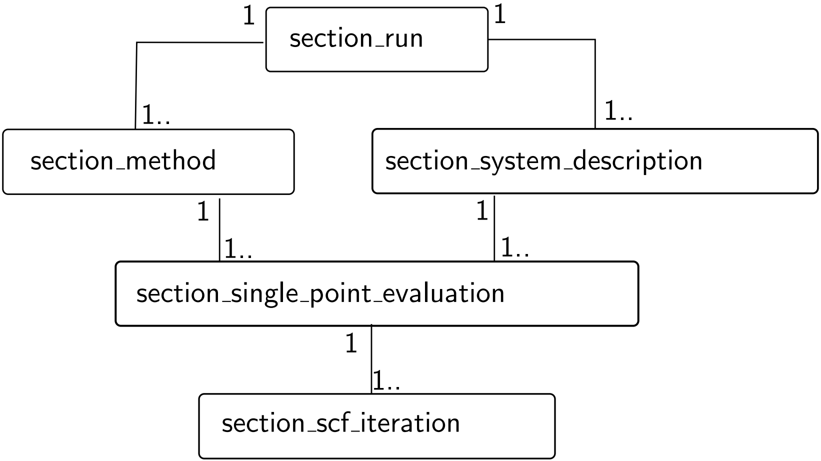

HOW STANDARDS PROLIFERATE:
(SEE: A/C CHARGERS, CHARACTER ENCODINGS, INSTANT MESSAGING, ETC)
SITUATION:
THERE ARE
14 COMPETING
STANDARDS.
14?! RIDICULOUS!
WE NEED TO DEVELOP
ONE UNIVERSAL STANDARD
THAT COVERS EVERYONE'S
USE CASES.
YEAH!
SOON:
SITUATION:
THERE ARE
15 COMPETING
STANDARDS.

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

NOVEL MATERIALS DISCOVERY

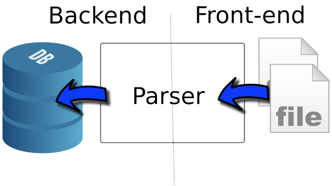
Common meta data: how to describe code independent quantities



What did we learn on parsers

- parsers should be fast because we want to apply them to large quantities of data (and re-parse regularly)
- parsers should be usable in various contexts
- code change in time, parsers need to evolve
- we will maintain and improve them for a while

Decoupling the parsers



- Independent systems are more robust
- can be changed or optimized independently
- can be reused in different contexts
- but the interface has to be chosen carefully, because it will dictate performance and complexity

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The simplest kind of efficient parser

- push parser
- call back based
- can stream (avoids loading everything in memory)
- main problem:
- you cannot tell the parser to skip some info
- solve this by adding the possibility to tell the parser about which info you are interested in

The dangers of freedom

- what is not seen by parsers is not seen by analysis
- data reliability is one of the most challenging problems
- we do not want throwaway parsers, parsers should detect subtle problems
  - did the program encounter a strange situation during convergence
  - where there warnings? Do they get propagated or is it just a line somewhere in the output
  - where there multiple runs in the same file? are they detected correctly?
  - ...and in the same directory? Are ancillary files really associated with the current run? What do creation dates say?...
  - contact with the code developers can help

declarative parsers

- try to describe the information that will be extracted
- we already have a way to do that: the meta data, we can extend it to describe code specific things too
- try to describe where to extract it
- example FHI-aims parser v3 written in python
- describe what should be done, but not how to do it: several ways to compile it into a real parser: adaptable and efficient
- close to documenting the thing to be parsed
- simpler for another person to change or optimize the parser (more optimization potential)

Declarative parsers problems

- difficult to describe transformations declaratively
- can be more tedious to write
- can be more difficult to debug (supporting tools can help here)
- possible solutions:
  - many derived quantities (like the normalized values) can be calculated at the section closing with a bit of caching
  - more complex normalization can be performed by another program.

The ideal parser

- starts with a declarative parser capable of parsing basically all information contained in an output
- optimizes it to extract the quantities required to calculate the code independent representation
- calculate the code independent quantities and return them
- can be reused in different contexts
- we can later decide that a quantity we ignored is now of interest.

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Conversion layer: not only parsers

- meta data tools
- getting raw data to parse, unique identifiers
- uncompress, find out which parser to use
- try to keep parsers minimal $\rightarrow$ common transformation in normalization step
- URI and interface to access pieces of data
- DB for meta data and references

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Identifiers

- identifier (gid) uses a small prefix (depending on what was checksummed) + the first 28 characters (168 bits) of the base64 encoding of the SHA-512 digest to identify most things (files, metadata, normalized data…)
- this allows one to build uri (`nmd://gid/path`) that refer to single quantities, or files within an archive
- uri do not depend on where the file is stored: ready for distributed approach

NOVEL MATERIALS DISCOVERY

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