VAMDC technology

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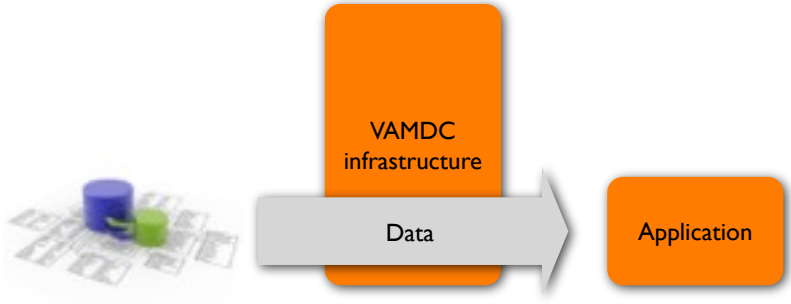
Innsbruck, February 2013


VAMDC
infrastructure
Data
Application

Plan A

Dump each database into a file and put on web.

Pro:

- "The simplest thing that could possibly work"
- Everything you can get has its own URL

Con:

- Data-sets too large (up to 10GB)
- No easy way to make data extracts

Plan B

Pre-compute all possible data extracts and dump on web

Pro:

- Selection now easy
- One URL for each possible extract

Con:

- Impossible to implement!

Plan C

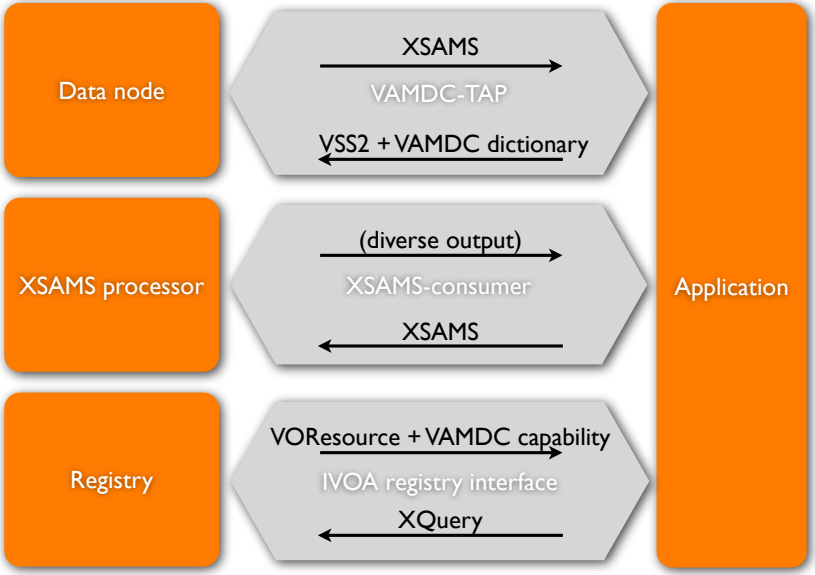
Compute data extracts on demand

but

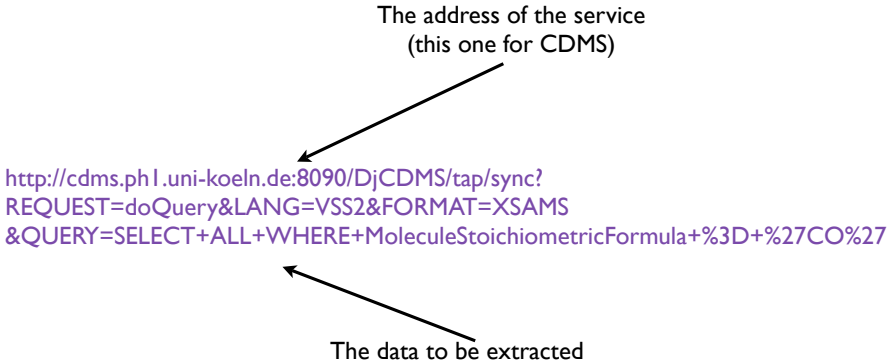
index them on the web as if pre-computed

- Pro:
  - Implementation now feasible
  - Still have a URL for every data-extract
- Con:
  - Some assembly required
  - Need to define standards for services, queries etc.

The core standards



Data URLs

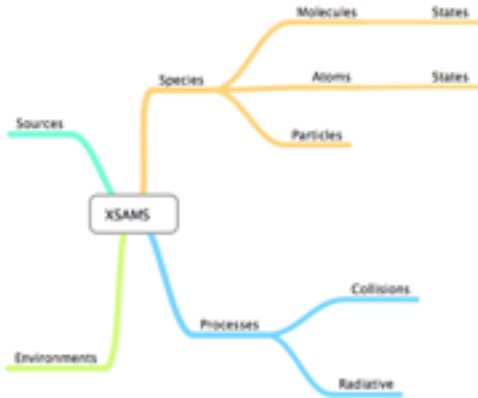


Call these with HTTP GET

XSAMS

- "XML schema for Atoms, Molecules & Solids"
- Developed by IAEA & VAMDC:
  - Proposed 2003, at IAEA DCN meeting
  - First versions by (IAEA, NIST, ORNL U. Pierre & Marie Curie, OPM, RFNC-VNIITF)
  - Subsequent development by VAMDC
- See http://www-amdis.iaea.org/xsams/
- See also http://www.vamdc.org/documents/standards/#data-model

XSAMS structure: top



XSAMS structure: bottom

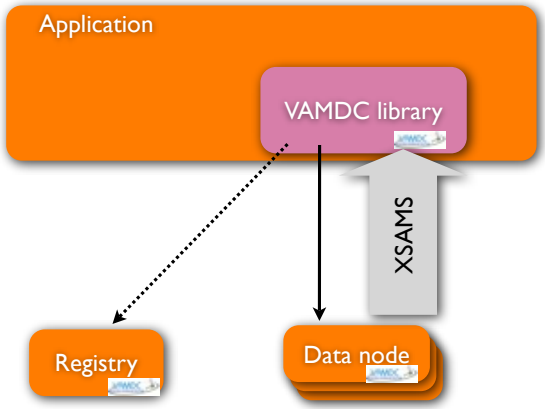
- All quantities have units
- All values can have associated uncertainties
- All values can have a source reference
- XML ⇒ no encoding issues for numbers

XSAMS for molecules

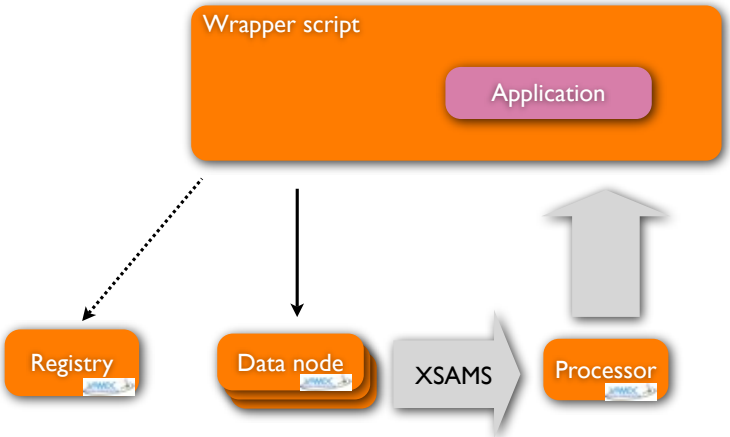
- "Case-by-case" XSAMS:
- Separate, additional schema for each class of molecule:

- 1. Diatomic closed shell (`dcs`): CO, N2, NO+
- 2. Hund's case (a) diatomics (`hunda`): NO, OH [for low J]
- 3. Hund's case (b) diatomics (`hundb`): O2, OH [for high J]
- 4. Closed-shell, linear triatomic molecules (`ltcs`): CO2, HCN
- ...etc up to at least 12 cases

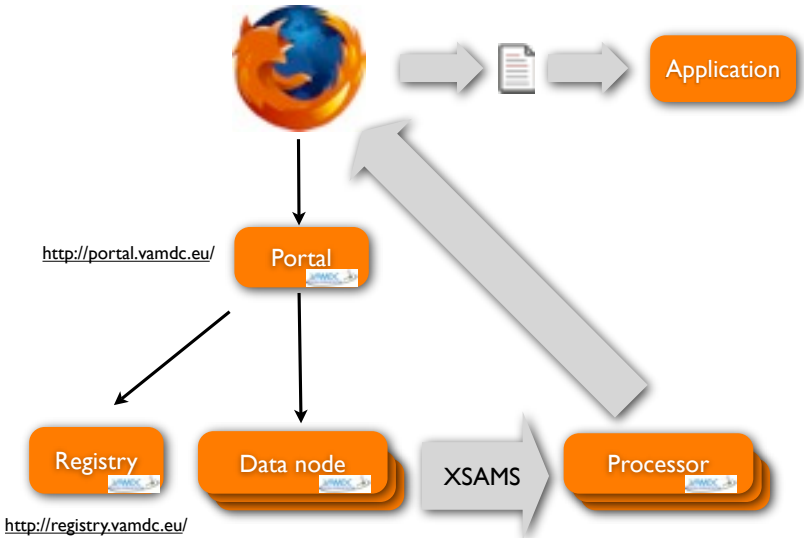
Adapted application



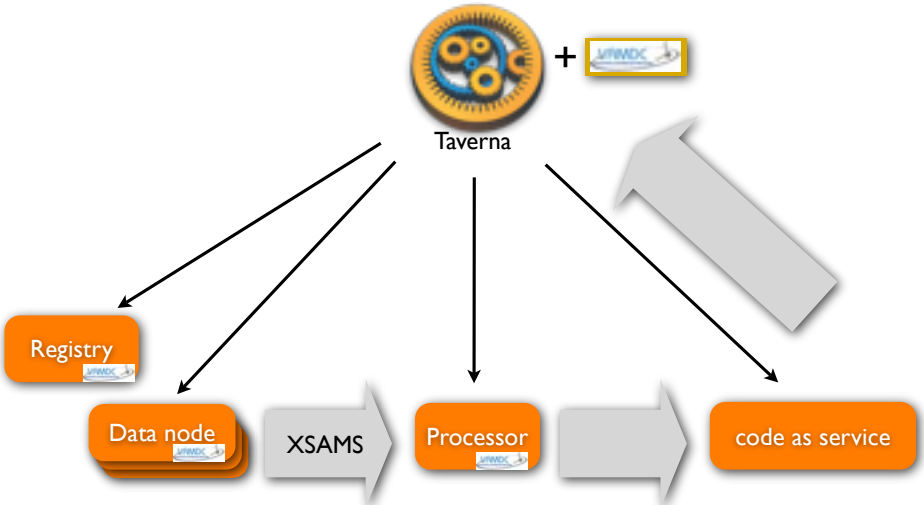
Wrapped application



Portal, nodes & processors



Taverna; code as service

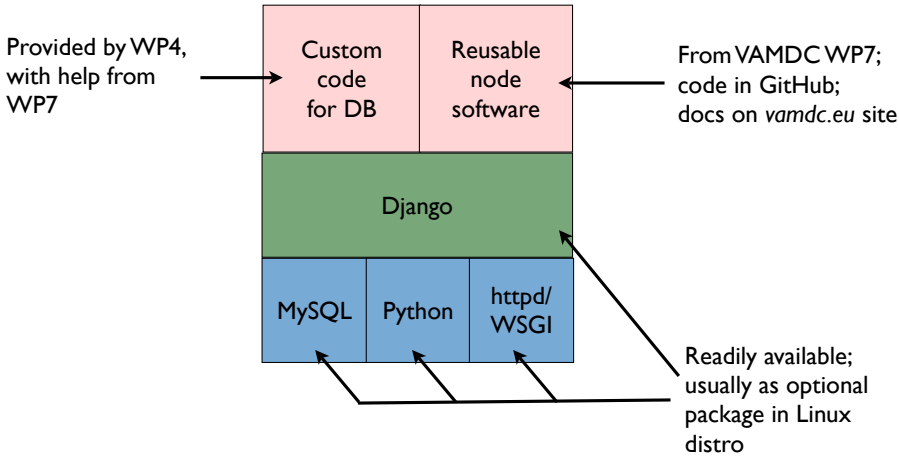


So how do I make a node?

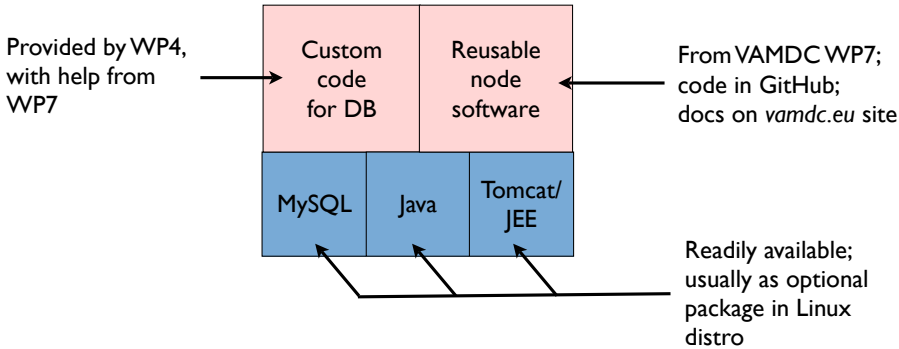
(And will it hurt?)

Node = database + web server + node software

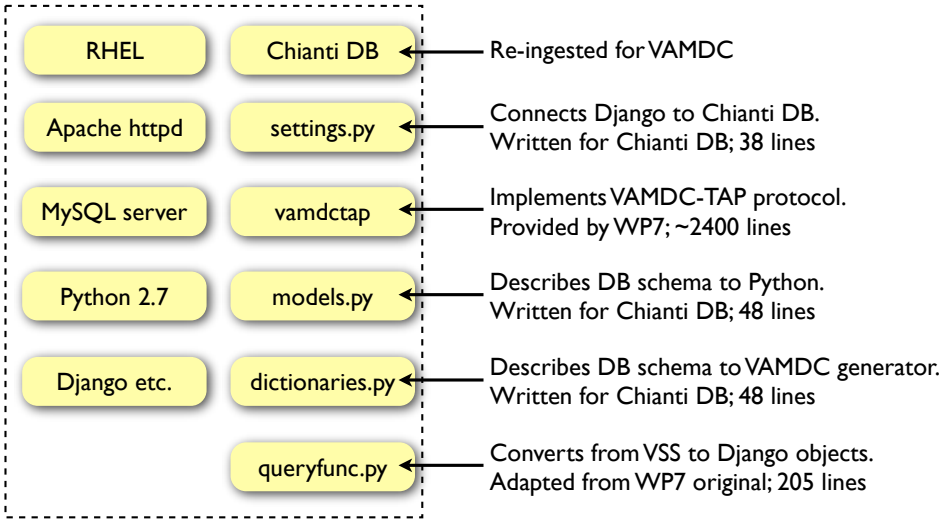
Node software in Python



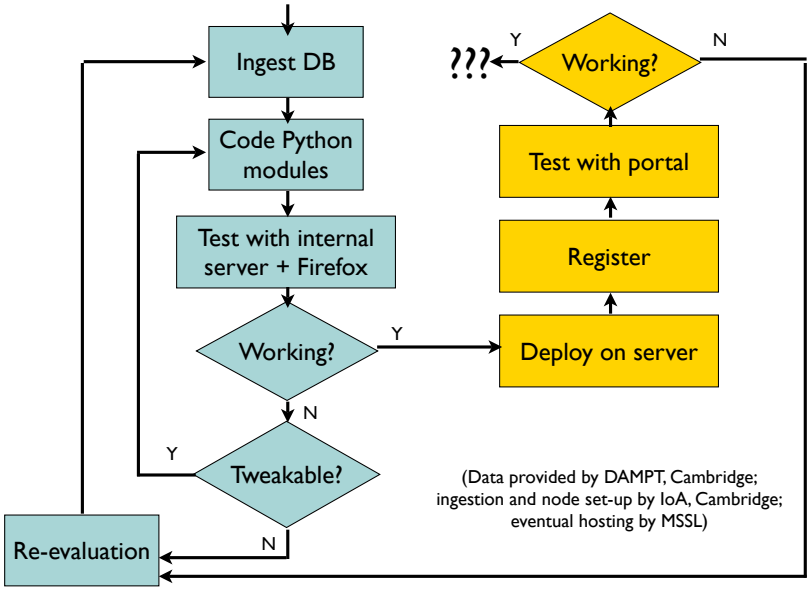
Node software in Java



Node example: Chianti



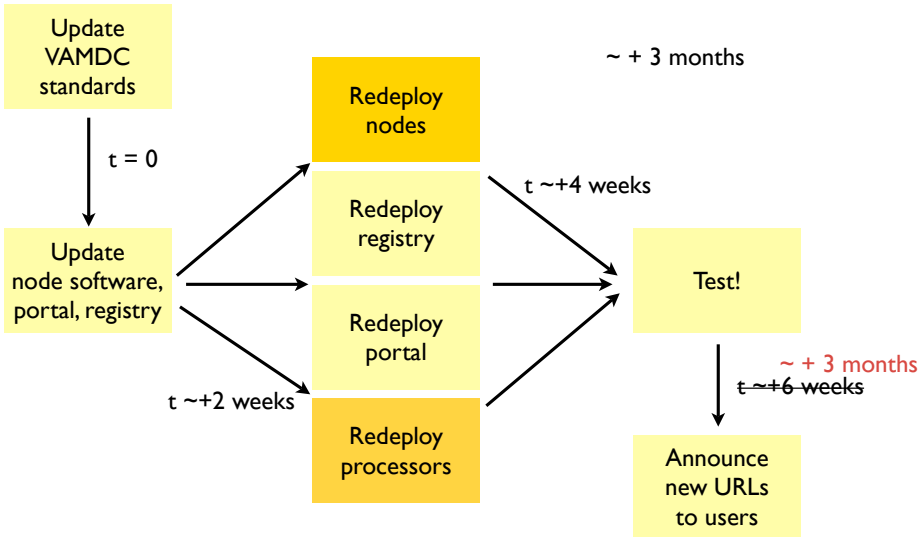
Chianti example (cont.)



System versions

- System version defined by standards version
- Three so far:
  - 11.05 (withdrawn)
  - 11.12 (current, released)
  - 12.07 (in preparation, to be released in 2013)
- Expect one new version per year from now on
- new standards ⇒ new deployments on new URLs

Annual updates of standards



Timeline of node registrations