

# OpenBIS pilot phase @ Concrete/Construction Chemistry Lab

Michele Griffa<sup>1</sup>, Janis Justs<sup>1</sup> , Nikolajs Toropovs<sup>1</sup>

<sup>1</sup> Concrete/Construction Chemistry Laboratory,

Swiss Federal Laboratories for Materials Science and Technology (Empa), ETH Domain

# Summary data

- Pilot phase start: 13. January 2020

- People involved:



Michele Griffa  
(data mining)




Janis Justs  
(labs management)



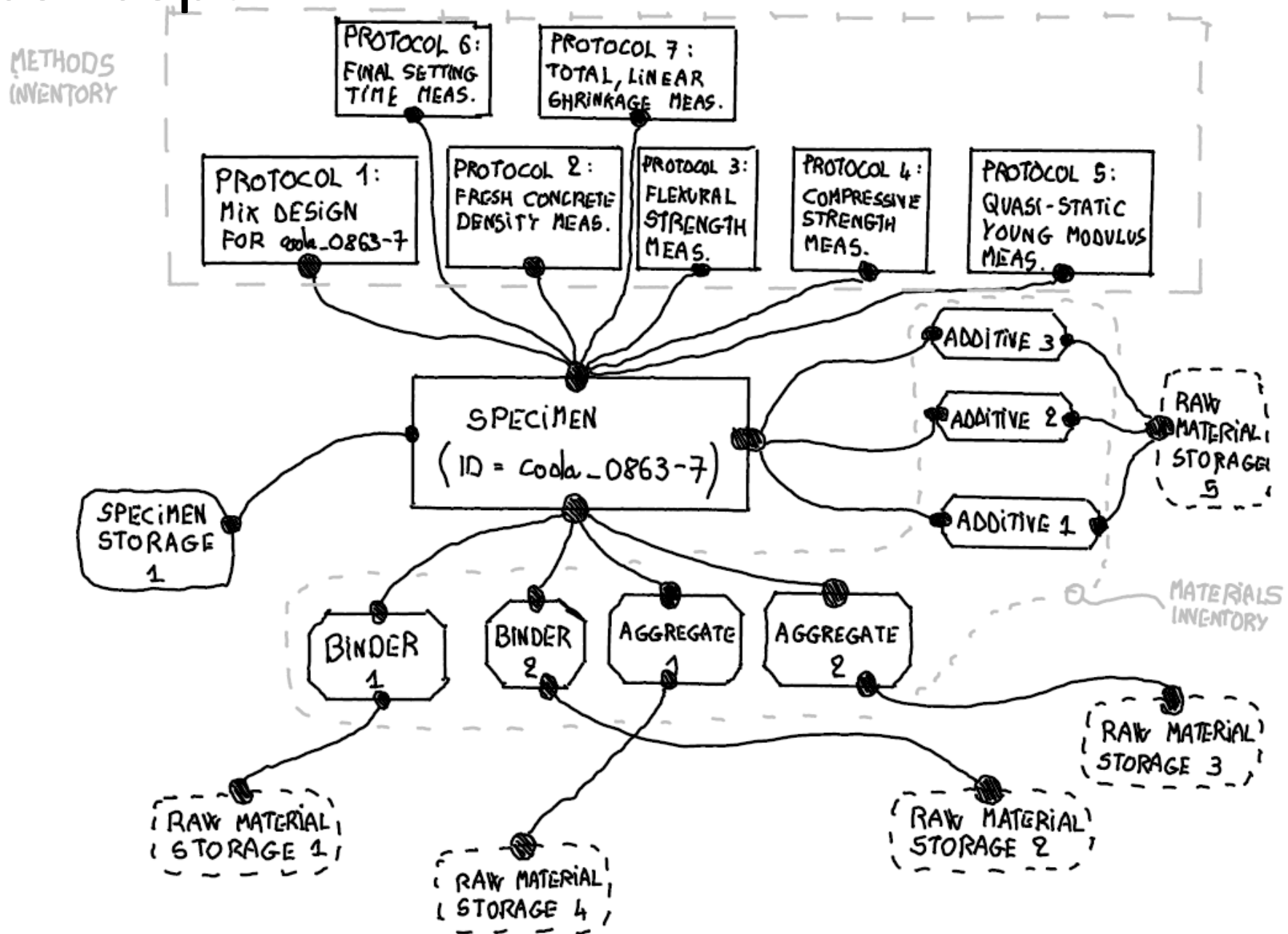
Nikolaj Toropovs  
(measurements)

- Cumulative man-hours (up to 23. Febr.): 132

# Starting concept

- Offer users predefined data structures/data for
    - measurement protocols
    - measured data
    - lab instruments and equipment
    - raw materials for specimens
  - Start with an example of extensive dataset from one specific project
  - Focus only on experiments
  - Build upon pre-existing data structures (creep/shrinkage data mining project in collaboration with BASF)
- 
- OpenBIS inventories

# Starting concept



## Actual implementation in OpenBIS: live demo

Object Hierarchy Graph for /TON/CODA/SAMPLE\_1

Filters Children: Parents: Show Types: 9 selected

The graph illustrates the hierarchical structure of a sample. At the top level, five parent objects are shown: ADMIXTURE:ADM3(No. W.A. 130), AGGREGATES:AGG1(Betriebssand 0-1), AGGREGATES:AGG2(Betriebssand 1-2), CEMENT:CEM3(i. work TE CNO CEM), and WATER:WATER\_1(Tap water). These parents lead to a central node, MIX\_DESIGN:CODA\_100\_0\_OPC\_CSA(100/0 OPC/CSA), which is highlighted in green. This central node further branches into two main categories: MASS\_LOSS\_MEASUREMENT and SHRINKAGE\_MEASUREMENT. Each category contains a series of numbered measurements, from 1 to 27 for mass loss and 1 to 6 for shrinkage. The graph is displayed in a web browser window with a sidebar showing a file hierarchy and a search bar.

```
graph TD; ADMIXTURE[ADMIXTURE:ADM3(No. W.A. 130)] --> MIX_DESIGN[MIX_DESIGN:CODA_100_0_OPC_CSA(100/0 OPC/CSA)]; AGGREGATES1[AGGREGATES:AGG1(Betriebssand 0-1)] --> MIX_DESIGN; AGGREGATES2[AGGREGATES:AGG2(Betriebssand 1-2)] --> MIX_DESIGN; CEMENT[CEMENT:CEM3(i. work TE CNO CEM)] --> MIX_DESIGN; WATER[WATER:WATER_1(Tap water)] --> MIX_DESIGN; MIX_DESIGN --> MASS_LOSS_1[MASS_LOSS_MEASUREMENT:MASS_LOSS_MEASUREMENT_1]; MIX_DESIGN --> SHRINKAGE_1[SHRINKAGE_MEASUREMENT:SHRINKAGE_MEASUREMENT_1]; MASS_LOSS_1 --> MASS_LOSS_3[MASS_LOSS_MEASUREMENT:MASS_LOSS_MEASUREMENT_3]; MASS_LOSS_3 --> MASS_LOSS_4[MASS_LOSS_MEASUREMENT:MASS_LOSS_MEASUREMENT_4]; MASS_LOSS_4 --> MASS_LOSS_5[MASS_LOSS_MEASUREMENT:MASS_LOSS_MEASUREMENT_5]; MASS_LOSS_5 --> MASS_LOSS_6[MASS_LOSS_MEASUREMENT:MASS_LOSS_MEASUREMENT_6]; MASS_LOSS_6 --> MASS_LOSS_27[MASS_LOSS_MEASUREMENT:MASS_LOSS_MEASUREMENT_27]; SHRINKAGE_1 --> SHRINKAGE_3[SHRINKAGE_MEASUREMENT:SHRINKAGE_MEASUREMENT_3]; SHRINKAGE_3 --> SHRINKAGE_4[SHRINKAGE_MEASUREMENT:SHRINKAGE_MEASUREMENT_4]; SHRINKAGE_4 --> SHRINKAGE_5[SHRINKAGE_MEASUREMENT:SHRINKAGE_MEASUREMENT_5]; SHRINKAGE_5 --> SHRINKAGE_6[SHRINKAGE_MEASUREMENT:SHRINKAGE_MEASUREMENT_6];
```

# Feedbacks to Empa/ETHZ

- Can OpenBIS be extensively customized for the Materials Science and Engineering fields?
- Is the customization easy and the learning curve with low gradient?
- Does a Lab need a programming geek to start to use OpenBIS?
- Do we urgently/necessarily need large scale data storage associated with the OpenBIS instance?
- Do we want to roll out OpenBIS for managing/supporting the Lab's research activities fast?

Yes!

Have no doubt about it!

Yes but ... expect some intense thinking about your daily operations!

No (if an Empa community of OpenBIS geeks is fostered!)

No! For the time being, metadata have priority

Absolutely yes!

# Plan for the future (till end 2020)

- Expand the data structure developed so far
- Pilot testing with two PhD student projects
- Test the Java/Python/Matlab APIs for
  1. simple plotting of stored data
  2. programmatic report generation from logged data and metadata
  3. programmatic data streaming from (a) few lab instruments to OpenBIS objects