



Simplifying Progress

WG Sample Prep: Introduction & Status

Allotrope Connect Virtual Workshop Spring 2020

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SARTORIUS

Agenda

Working Group Sample Prep introduction

Scope definition

Unit Operation: Model for data structuring

D-SI: Standard format for measure values

Conclusion



WG Sample Prep: Members

- Reinhard Baumfalk, Sartorius (WG Lead)
- Pasi Kankaanpaa, Sartorius
- Thomas Schink, Sartorius
- Holger Linnerz, Mettler Toledo
- Gerald Hall, Agilent
- Heiko Fessnmayr, Agilent
- Hossein Arjomand, Thermo Fisher
- Matthew Fox, ALLOTROPE
- Christoph Schaub, Bayer
- Raghu Arrola, Astra Zeneca
- Wolfgang Colsmann, Osthus
- Helge Krieg, Osthus
- ... are still open for more



SARTORIUS



Agilent Technologies



ThermoFisher
SCIENTIFIC



WG Sample Prep: Status

- Model for data definition finalized
- Review with ALLOTROPE Modelling group / Architects ongoing
- Prototypes for examination Unit Operation concept in preparation (Sartorius, Agilent)

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Sample Prep: some Impressions (what do we understand talking about sample prep)



Sample Prep: Definition

Wikipedia:

In analytical chemistry, **sample preparation** refers to the ways in which a sample is treated prior to its analyses. Preparation is a very important step in most analytical techniques, because the techniques are often not responsive to the analyte in its in-situ form, or the results are distorted by interfering species.

Sample preparation may involve dissolution, extraction, reaction with some chemical species, pulverizing, treatment with a chelating agent (e.g. EDTA), masking, filtering, dilution, sub-sampling or many other techniques. Treatment is done to prepare the sample into a form ready for analysis by specified analytical equipment.

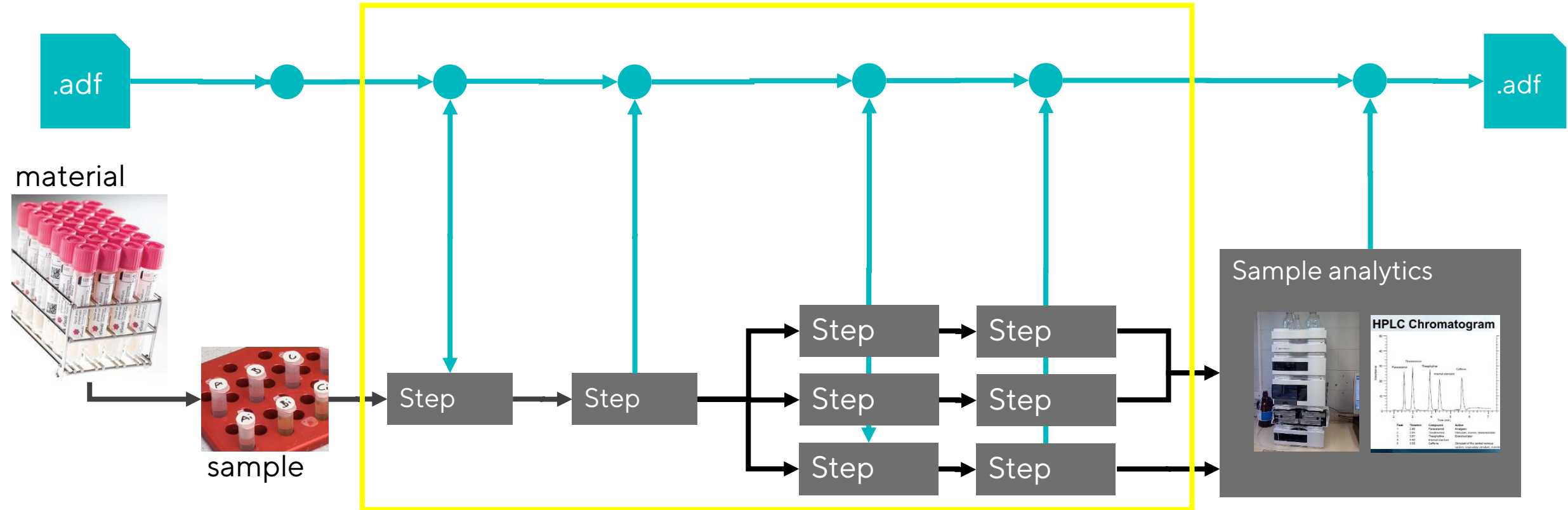
Sample preparation could involve: crushing and dissolution, chemical digestion with acid or alkali, sample extraction, sample clean up and sample pre-concentration.

Source: <https://en.wikipedia.org>

Allotrope WG:

Needed information to ensure completeness of analytical data (sample prep and analysis) and to improve quality of data analytics.

Scope for sample prep WG



Requirements for documentation: Stakeholder view

Scientist

- Reliability in analytical results
- Traceability of results
- Comparability of results

Lab Manager

- Execution quality
- Flexibility in protocol execution
- Lab work optimization

Pharma Manufacturer

- Development speed
- Efficiency

Lab IT

- Consistent, safe, secure data management
- Completeness of data
- Easy access to all collected data

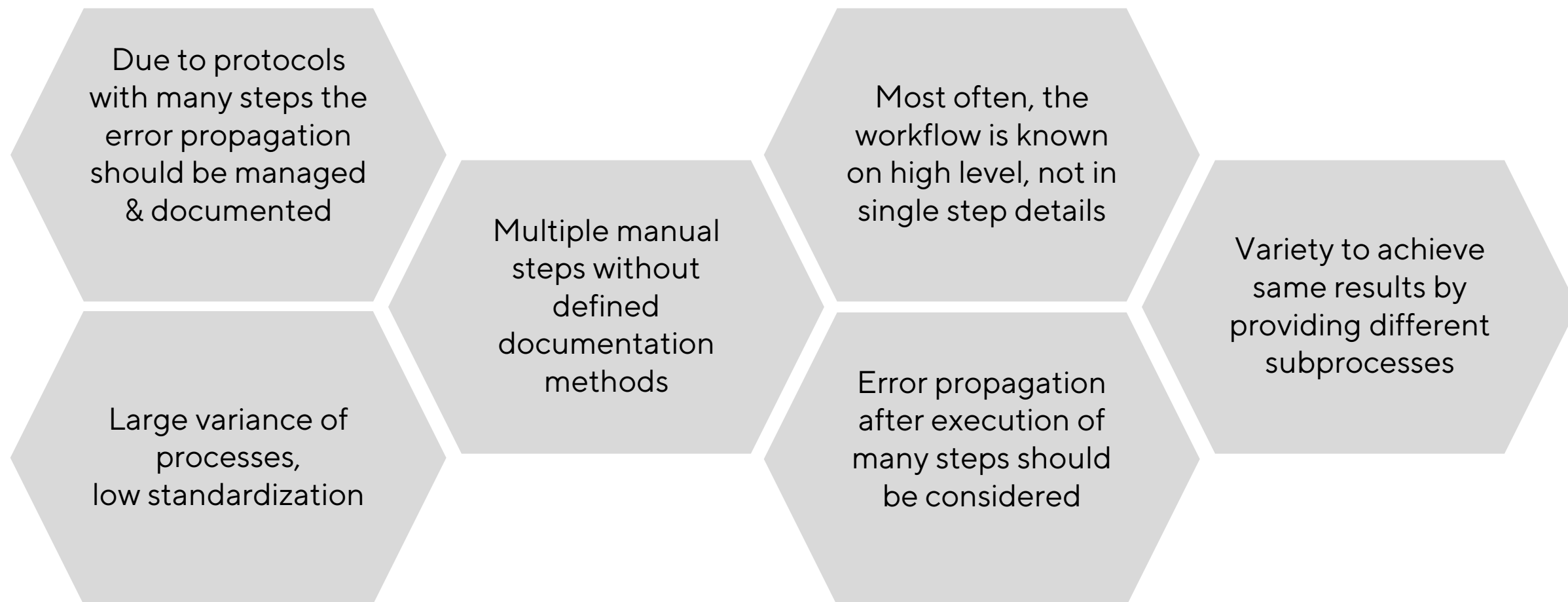
IT integrator

- Easy to integrate all kind of lab equipment
- Buildup domain specific network & data structures

Asset supplier

- Provide easy to use lab solutions
- Establish new solutions to make lab work easier
- Ensure the proper use of assets

Challenges for Sample Prep workflow documentation



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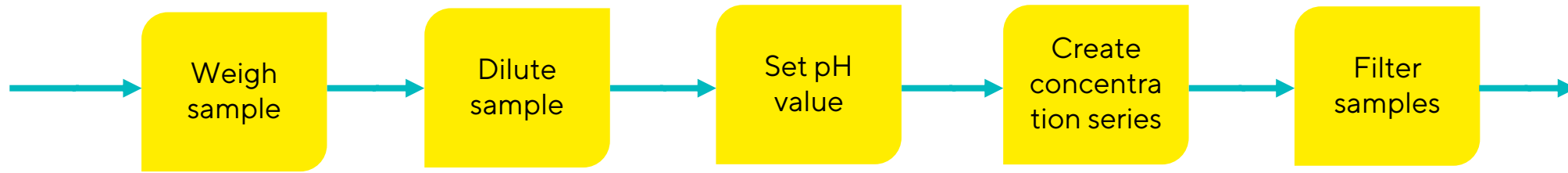
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Sample Prep: WG concept

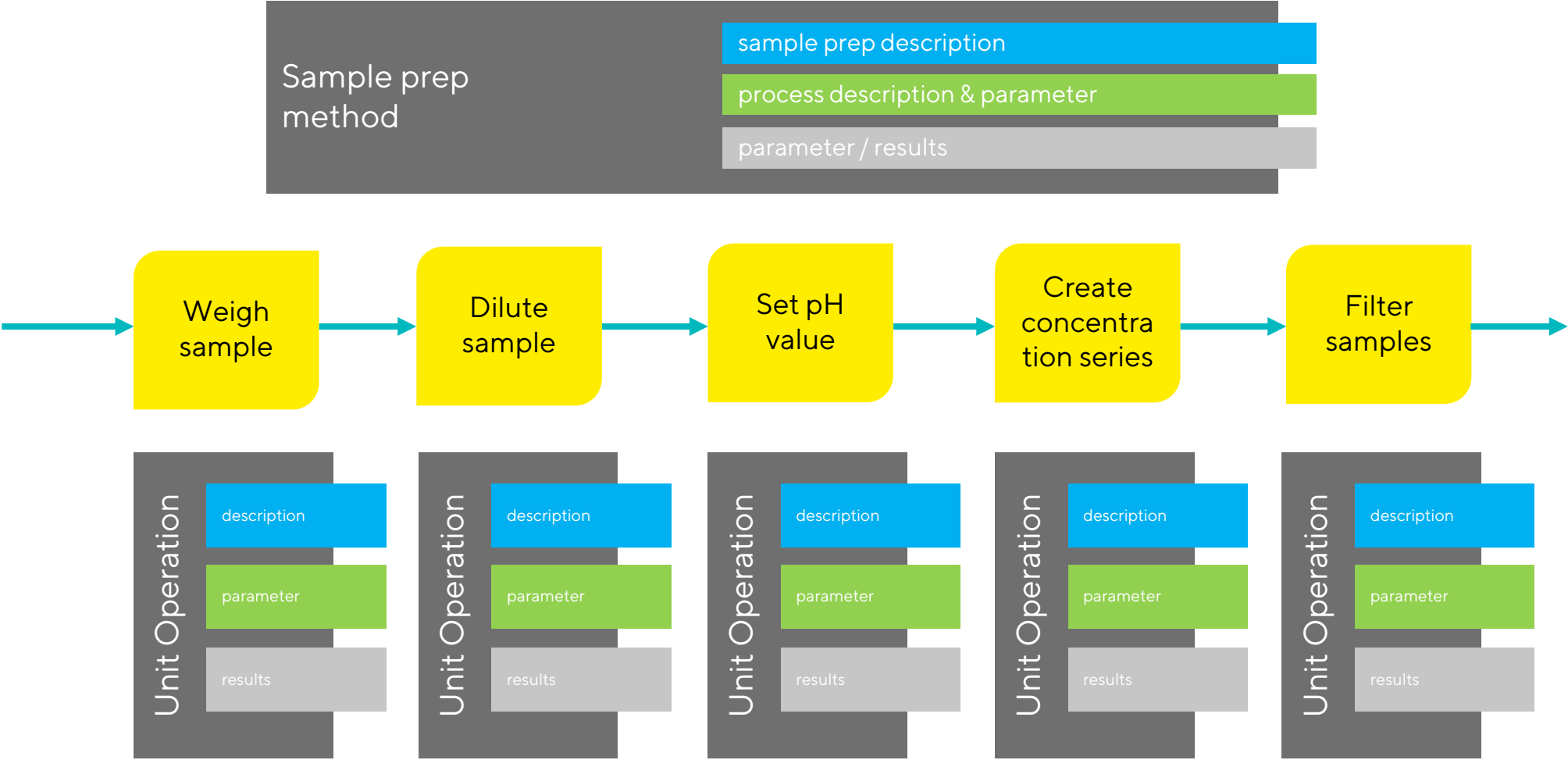
Sample Preparation for Analytic (e.g. HPLC, ...):



For a Lab scientist/technician this workflow is sufficient, gives on a high level enough information but:

- Each step consists of sub steps
- For execution of these steps different instruments, tooling, assets, ingredients are needed. These can differ from lab to lab, lab technician, stock, ...
- Execution of the steps and the sub steps are depending on the lab technician's experience.
- Documentation of the actual execution is not done in most cases

Concept “Unit Operation” for elementary lab processes



Modelling elements for lab work

Sample Prep Workflow:

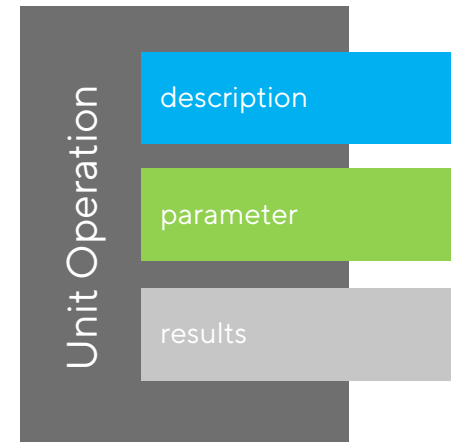
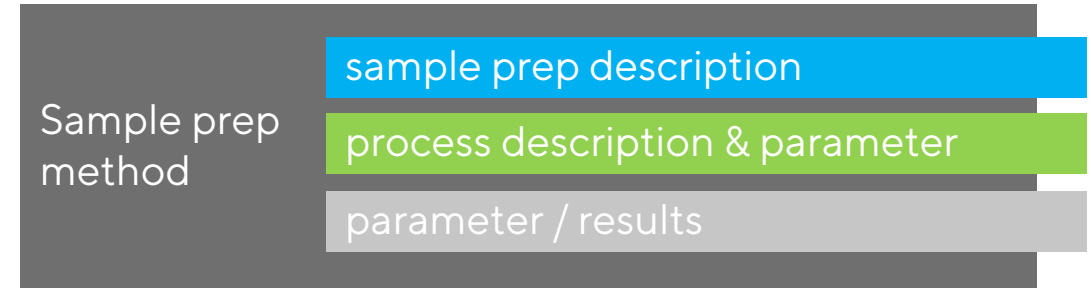
Consists of a sequence of elementary services (Unit Operations).

Defines and / or documents the executed process as a composition of Unit Operations.

Unit Operation:

a digital representation of an elementary lab process including data for

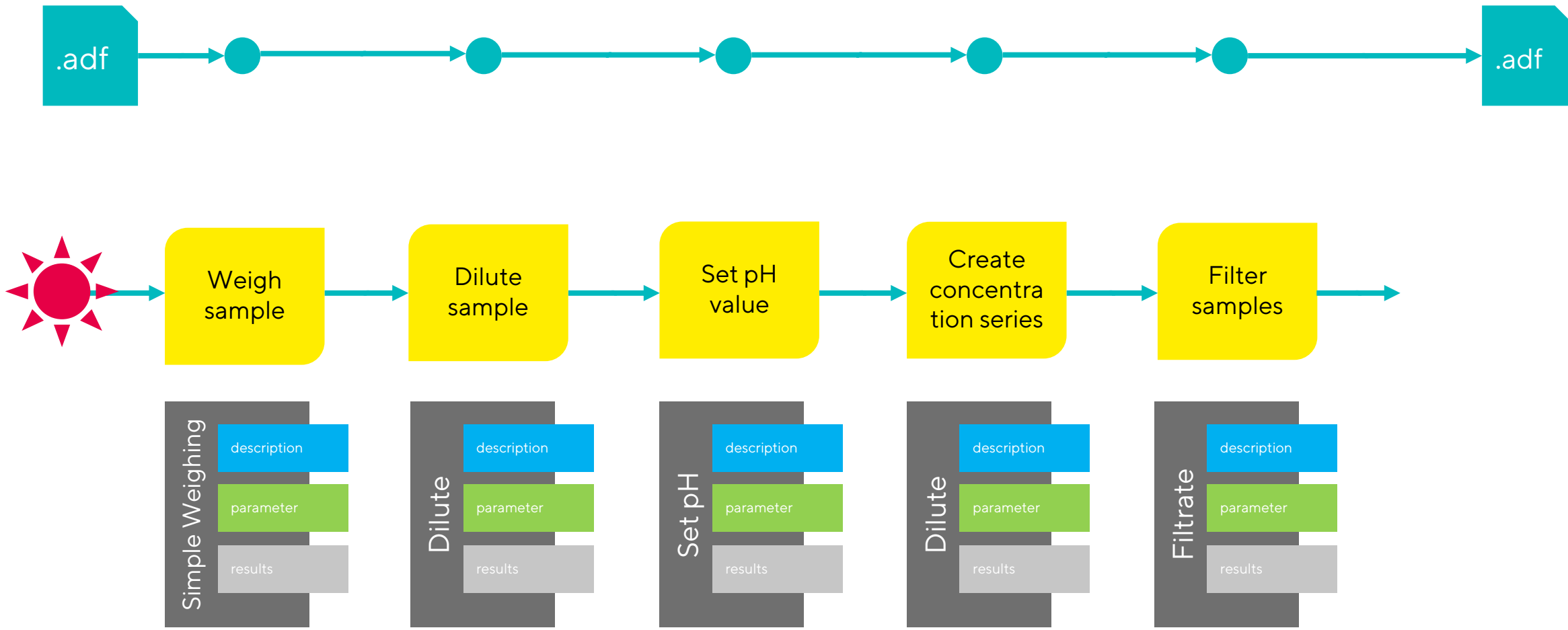
- workflow,
- used means (instruments & consumables),
- parameters
- achieved results



Unit Operation: Key benefits

- Sample prep workflow consists of a collection of Unit Operations, no additional detail on this level needed
- Workflow design and process documentation is based on lab perspective
- Provider of instruments and material to lab can provide Unit Operations to optimize the use of their products
- Structuring of data along services, not instruments
- Parameter and results are assigned to the service, not to the device
- Instruments mostly providing more than one workflow (application)
- Same structure for manual or instrument supported workflow can be used
- Flexibility is given for different types of instruments
- Lab automation can also be covered by the Unit Operation model

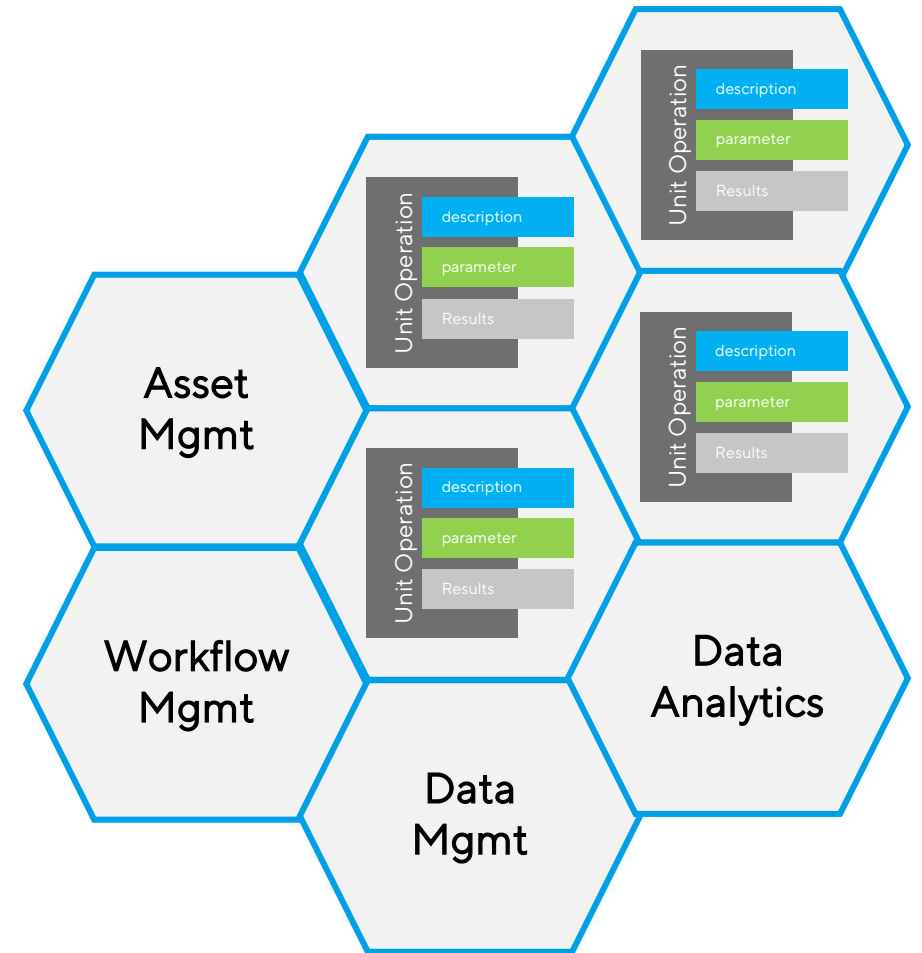
Use Case: Collecting UO data during execution



Use Case: Sample Prep in a managed lab

Unit Operation model could be a benefit of Lab IOT data architecture:

- Decentralized service structure
- Simple, flexible integration of lab components
- High quality data acquisition standards
- Flexible workflow design
- Full traceability of sample preparation work



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D-SI : Digital System of Units

The definition of a standard for measure data in the digital world is essential for the exchange of metrological information in all fields of Information and Communication Technologies (ICT).

In terms of content, the format considers essential international metrology guidelines and standards.

Publications:

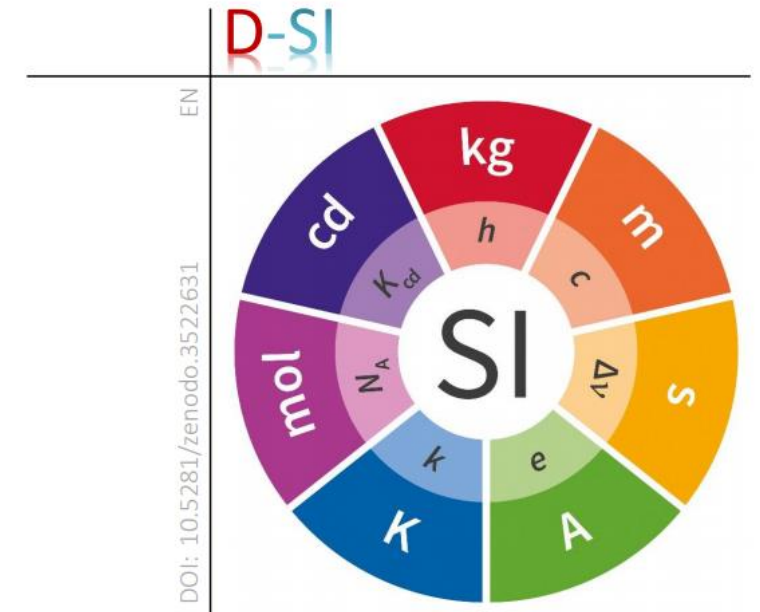
Universal format for transfer of metrological data via digital communications

- <https://doi.org/10.5281/zenodo.3522631>
- <https://doi.org/10.5281/zenodo.3522074>

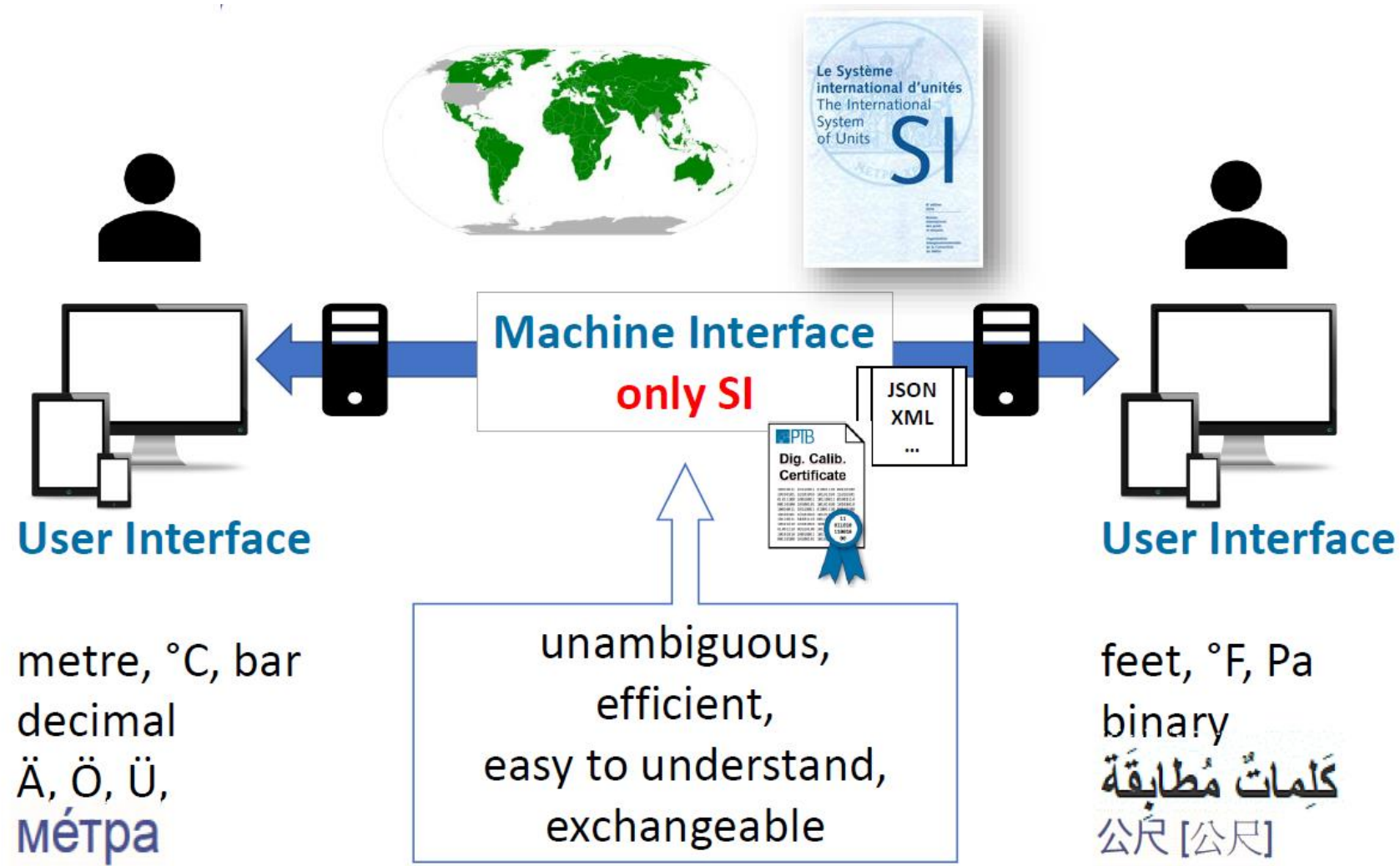
Digital System of Units

Digital Calibration Certificate

DCC – XML Schema



Use Case for D-SI



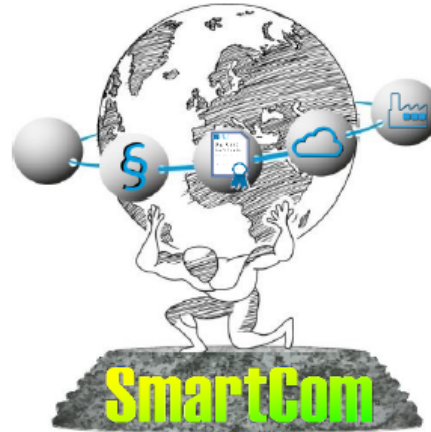
Digitalization for measure data is global ...

○ Contacts und cooperations in 2018



Key Objectives

- Digital SI Metadata Model (D-SI)
 - transfer of metrological data via digital communications
 - atomic and extended models
 - SI units vs. non-SI
- Digital Calibration Certificate (DCC)
 - standards like ISO 17025
 - secure transfer
 - Structure (administrative and measurement data)



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04/2020

D-SI: Real data model

$$Y = y \text{ [SI]} \pm U_{95}(k) \text{ distribution UTC}$$

constant quantity type	components (of the constant quantity type)					
	label	value	unit	dateTime	uncertainty	distribution
constant quantity with an exact value						
constant quantity with an uncertainty						

mandatory optional

```

<si:real>
  <si:value>2.34</si:value>
  <si:unit>\metre</si:unit>
  <si:label>length</si:label>
  <si:dateTime>2018-11-16T12:30:01.67-01:00</si:dateTime>
</si:real>

```

SI unit format

VIM

ISO 80000

IEEE 754

RFC 362 (UTF-8)

ISO 8601



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Conclusion

- Unit Operation concept for sample prep processes creates the opportunity
 - To bring up precision of analytical results
 - To Improve the quality of data (metrology)
 - To enable data analytics
- Unit Operation concept defines a concept
 - To cover the workflow, including manual work,
 - Acquire more information than the acquisition of pure measure data given by the used instruments.
 - Gives a definition for modelling workflows
- Unit Operation gives especially the sample preparation the potential to get a link to IOT
- Sample Prep is 1st example for ADF as input and output format (build data chains)
(IOT: “vertical & horizontal data exchange”)
- With the Digital-SI format definition for measure values
 - Gives an universal standard for measure values
(compared to the well established SI unit definitions)
 - Simplifies the management of calibration certificates of instruments (see DCC / DSI projects) by defining a common standard

Thank you.

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The Sartorius logo is displayed in a bold, black, sans-serif font. The letters are closely spaced, and the 'S' and 'A' are particularly prominent. The logo is centered on a bright yellow rectangular background.