BASF
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True Instrument Integration Requires More Standardization

Allotrope Spring Connect 2024

Sven Arenz

BASF – We create chemistry

- Our chemistry is used in almost all industries

- We combine economic success, social responsibility and environmental protection

- Sales 2023: €68.9 billion

- EBIT before special items 2023: €3.8 billion

- 111,991 Employees organized in 6 segments / 11 divisions (as of December 31, 2023)

- 6 Verbund sites and 234 other production sites

- Over 78,000 customers from various sectors in almost every country in the world

Chemicals

Materials

Industrial Solutions

Surface Technologies

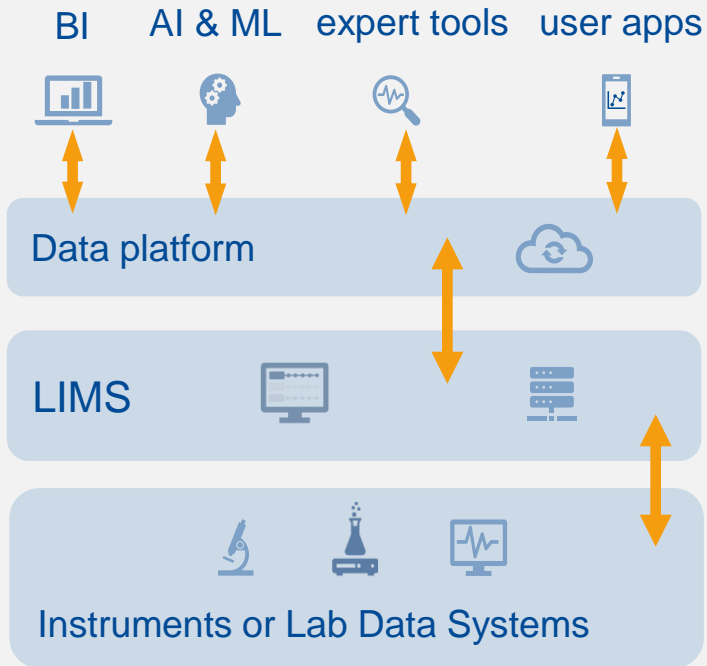Nutrition & Care

Agricultural Solutions

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Analytics creates Value

Role of Analytics

- Key Enabling Platform along all business processes and value chains

- Core of all knowledge-driven innovation

- Drives efficient and effective production processes and secures our license to operate

- Fundamental to digital transformation

Research • Production • Regulatory Affairs • EHS • Marketing

Internal

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LIMS: Data Center of an Analytical Lab

BI AI & ML expert tools user apps

Data platform

LIMS

Instruments or Lab Data Systems

To fully leverage the potential of data…

… a sustainable and efficient integration of instrument is essential

Data from more than **3000 instruments** (> 500 models, 150 vendors) need to be managed (collected, parsed and processed)

LabVantage Scientific Data Management System

✓ Indirect connection

✓ Generic file interface

✓ **Instrument specific data parsing and proccessing**

Evolution of Instrument Data Parsing and Processing

Connected instruments
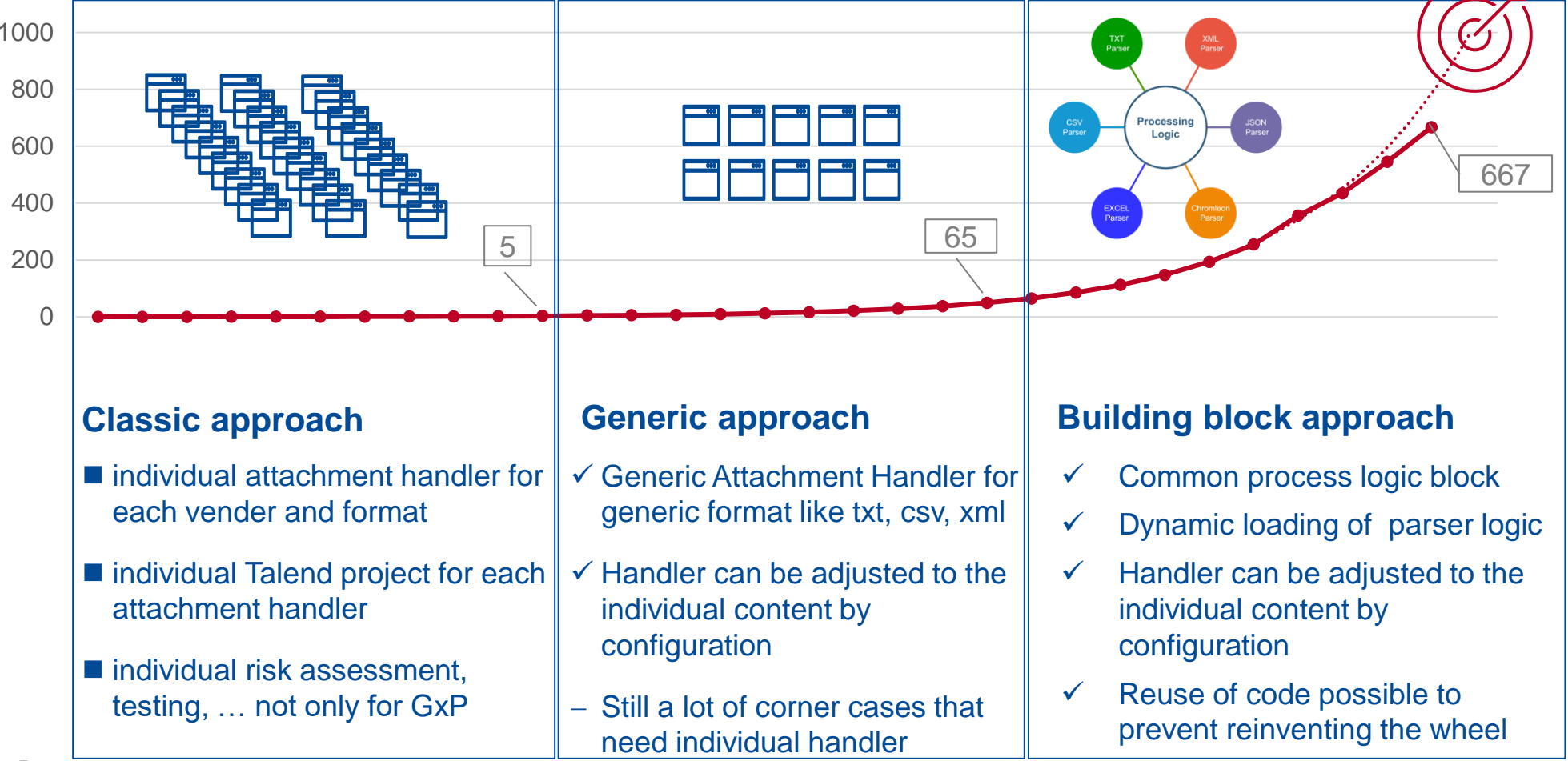
Most instruments can report data in generic format like txt, csv, xml…

Classic approach

- individual attachment handler for each vender and format

- individual Talend project for each attachment handler

- individual risk assessment, testing, … not only for GxP

Generic approach

✓ Generic Attachment Handler for generic format like txt, csv, xml

✓ Handler can be adjusted to the individual content by configuration

– Still a lot of corner cases that need individual handler

Building block approach

✓ Common process logic block

✓ Dynamic loading of parser logic

✓ Handler can be adjusted to the individual content by configuration

✓ Reuse of code possible to prevent reinventing the wheel

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What is needed for sustainable integration of lab instruments?
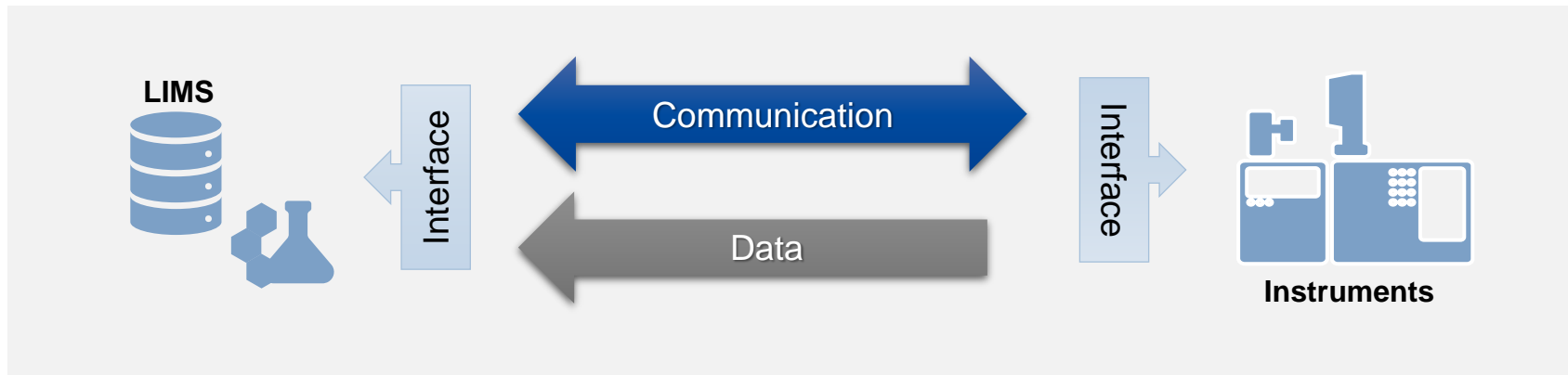
- Communication ➔ **Communication standards** (LADS/OPC-UA, SilA2)

  ▸ A Communication Protocol **alone** leaves us with proprietary data structures (data silos)

- Data Exchange ➔ **Data standards** (Allotrope, AniML, Frictionless)

  ▸ A Data (File) **alone** is not suitable for systems where components need to communicate

Internal

LADS – Laboratory Agnostic Device Standard
The SPECTARIS, VDMA & OPC-Foundation initiative

The goal of LADS is to create a manufacturer-independent, open standard for analytical and laboratory equipment that comprehensively reflects the different customer industries and their respective workflows.

LIMS — Interface — OPC-UA (LADS) — Lab-Data standard — Interface
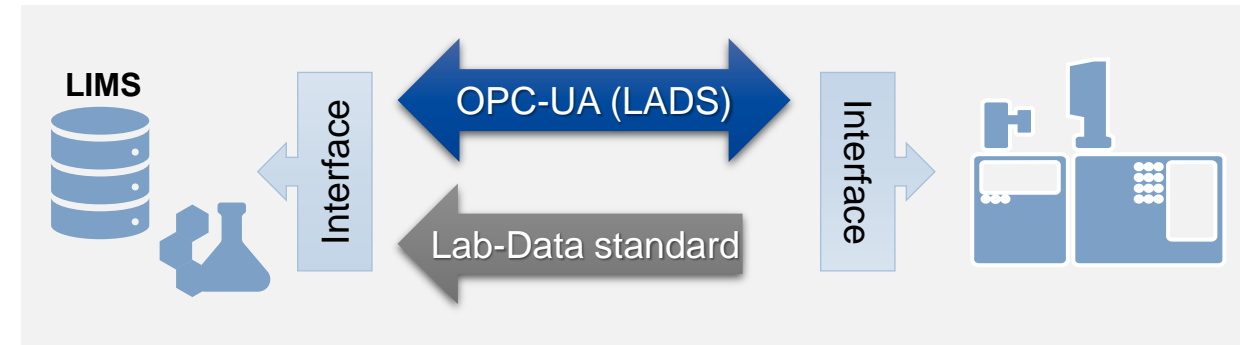
Build on proven Technology & Copy with Pride

- Utilize proven **OPC-UA** standard features & **Companion Specifications** whenever feasible

- Support existing **Lab-Data standards** (AnIML, Allotrope, ..)

Support Heterogeneity (Device, Vendor, App…)

- Follow device-type-agnostic design

https://www.spectaris.de/en/association/thespectarisindustries/networked-laboratory-equipment/

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LADS – "Hackathon" @ BASF

For two days BASF Analytical & Material Science hosted members of the innovative SPECTARIS standardization initiative OPC UA LADS.
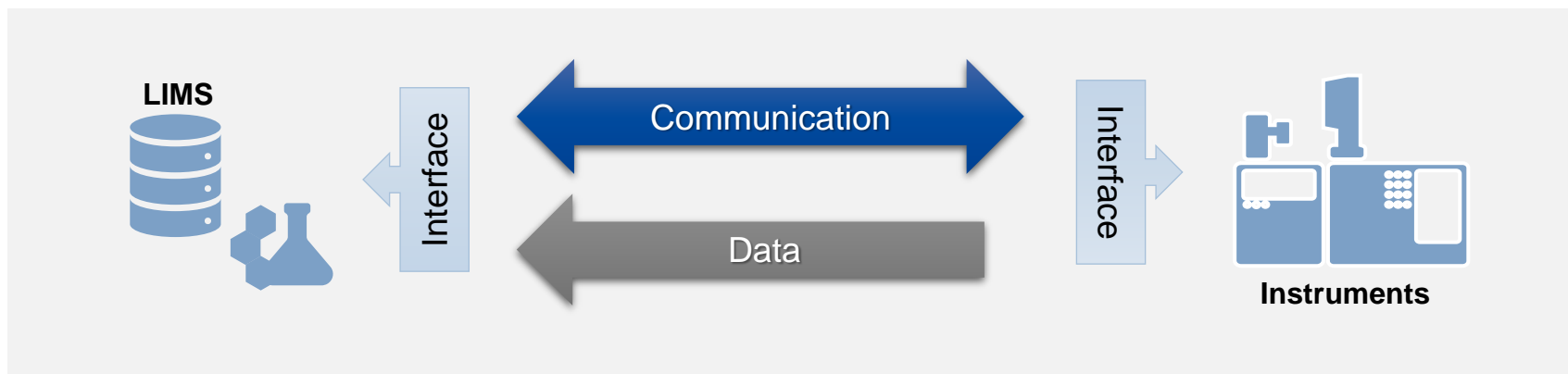

Matthias Arnold, Bruno Schliersmair, Jan Schmidle and Matthias Schuh were challenged by BASF lab digitalization experts from different departments.

The groups worked jointly on topics like brownfield connectivity, future-proof device modeling and LIMS & SDMS integration.

In agile programming sessions, the group even "hacked" viable solutions for several challenging scenarios.

https://www.linkedin.com/feed/update/urn:li:activity:6958575900787384320?updateEntityUrn=urn%3Ali%3Afs_feedUpdate%3A%28V2%2Curn%3Ali%3Aactivity%3A6958575900787384320%29

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True Integration Requires More Standardization

LIMS

Interface

Communication

Data

Interface

Instruments

Communication standard

➜ **OPC-UA**

Data standard ➜ Data Format Candidates Evaluation

? Snow white project with the goal to extend the experience in handling industry standards for laboratory data (AniML, Allotrope, Frictionless data) in BASF, building up knowledge to decide which format to use when, creating awareness of the libraries, tools and solutions available on the market to handle these data formats.

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Components of Complete Data Standards

Define → **Classify** → **Relate**

Vocabulary — Taxonomy — Ontology

Charter, Attribute 3, Person, Project, Roles, limits, limits, Department, Target, Team, Attribute 2, Person, Attribute 1

CSV ZIP JSON
HDF5 RDF XML

Context
Consistent use of preferred terms across lab data adds uniform context.

Structure
Data models are blueprints for use of preferred terms to describe lab items.

Format
Final standardized representation of structured data in software applications.

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https://www.allotrope.org/

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The Allotrope Framework

Defines terms & their relationships consistently across laboratory domains

Establishes schema for consistent use of ontologies to describe laboratory items

Provides standardized data format (RDF) to semantically represent laboratory data

Vendor Product → Modeling → Allotrope Modeling Toolchain

APPLY

VALIDATE | VIEW

GOVERNANCE

Prioritized use case → AFO Ontologies → ADM Data Models → STRUCTURE → RDF → ARCHIVE AND UNPACK & USE

MORE COMPLEX USE CASES
Expand a knowledge graph

APPLY

AUTOMATION

Enrich existing data with AFO

ASM Simple Models → STRUCTURE → JSON → USE

LESS COMPLEX USE CASES
Direct use in downstream applications, R, BI, Python, etc.

instrument integration

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ASM schemas are used to describe and validate the structure of an ASM instance

Provides standardized text-based representation (JSON) of laboratory data

https://www.allotrope.org/

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Evolution of Instrument Data Parsing and Processing

Allotrope approach

✓ Common process logic block

✓ Generic JSON parsing logic blocks

✓ Content parsing configuration is given by JSON schema

✓ Automates data instance validation by JSON schema

✓ Handler can be further adjusted to the by configuration

Sustainable integration of lab instruments requires standards …

JSON Schema

JSON Parser

Processing Logic

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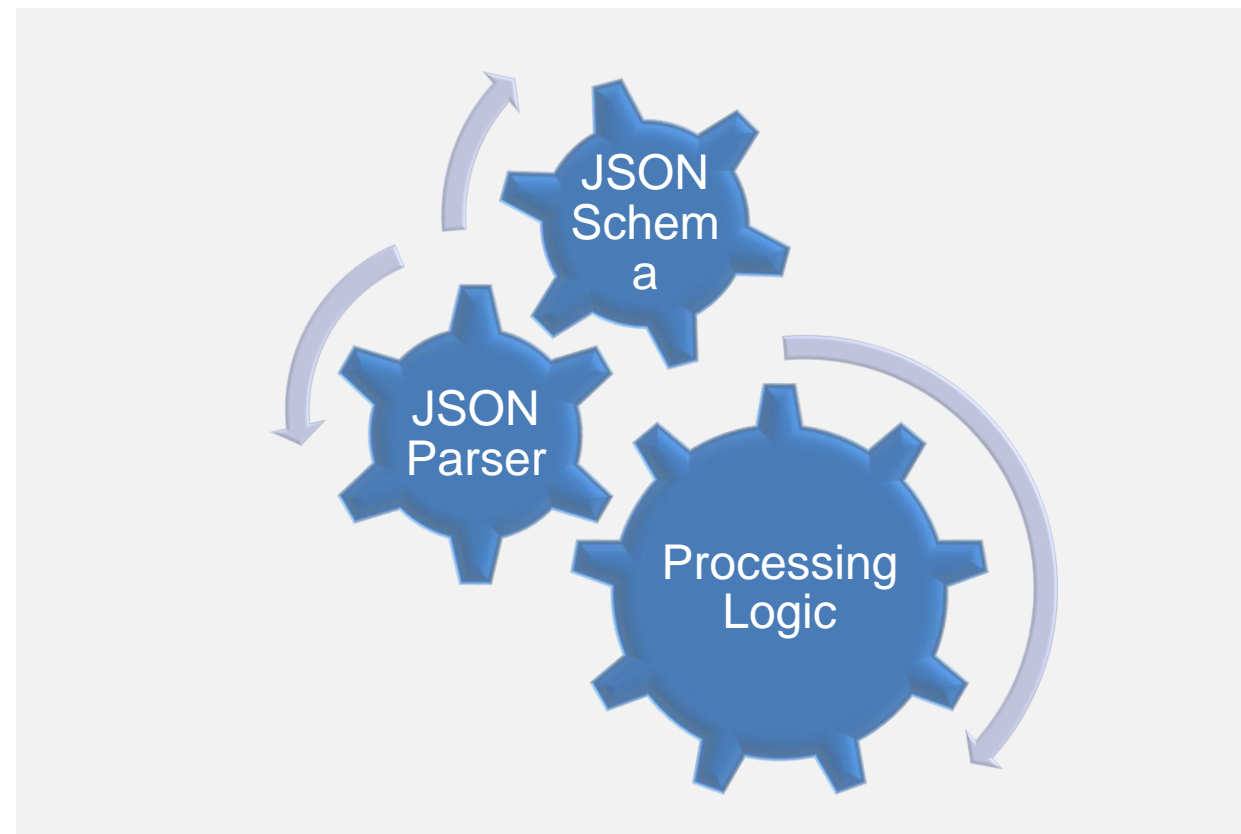
Mission Statement VisuAll

"From Instrument Data to Insights":

⊙ Intuitive Visualization of
Big Multidimensional Instrument Data

⊙ With Standardized, Verified Imports
from Labvantage to Foundry

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Instrument Datasets are Structured, but not Standardized

Big Multidimensional Instrument Datasets are for example:

- Force Curves, Rheology, IR Spectrum, TG-A, FTIR, Colorimetry, Color-Spectrum, GC, HPLC, Mercury Porosimetry

- Data only usable in vendor software
  - ▶ Vendor lock in for all data created by instrument
  - ▶ Standalone data, e.g. no relation to formulation data in LIMS

- Excel Export from vendor software exist, BUT
  - ▶ Different structure even for same instrument type
  - ▶ Datasets too large for direct import in LIMS

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Vizualizing Big Multidimensional Dataset is creating insights

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LIMS: Data Center of an Analytical Lab

Palantir Foundry

Scaleable Adaptive Visualization
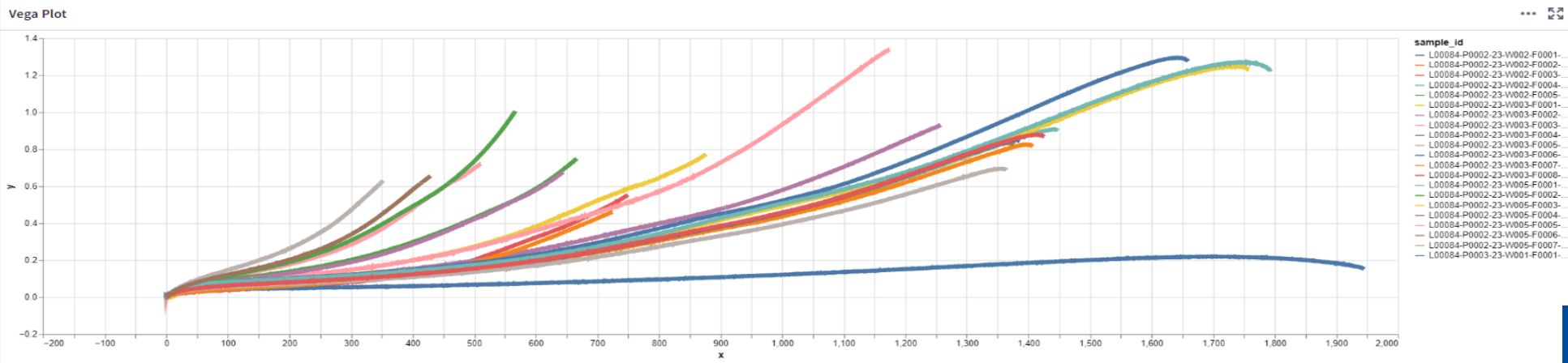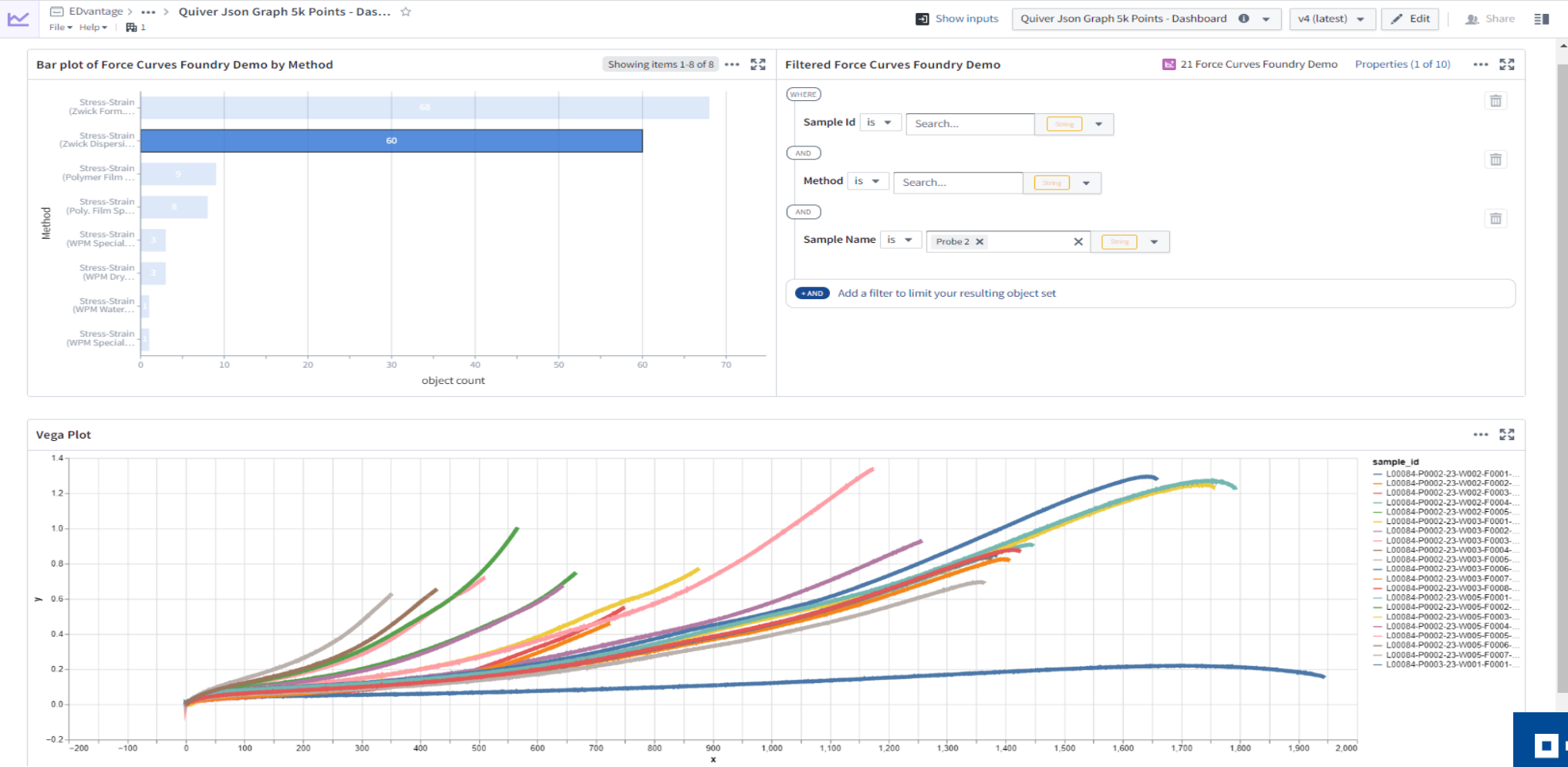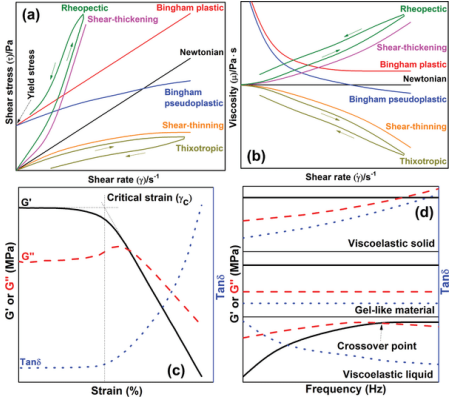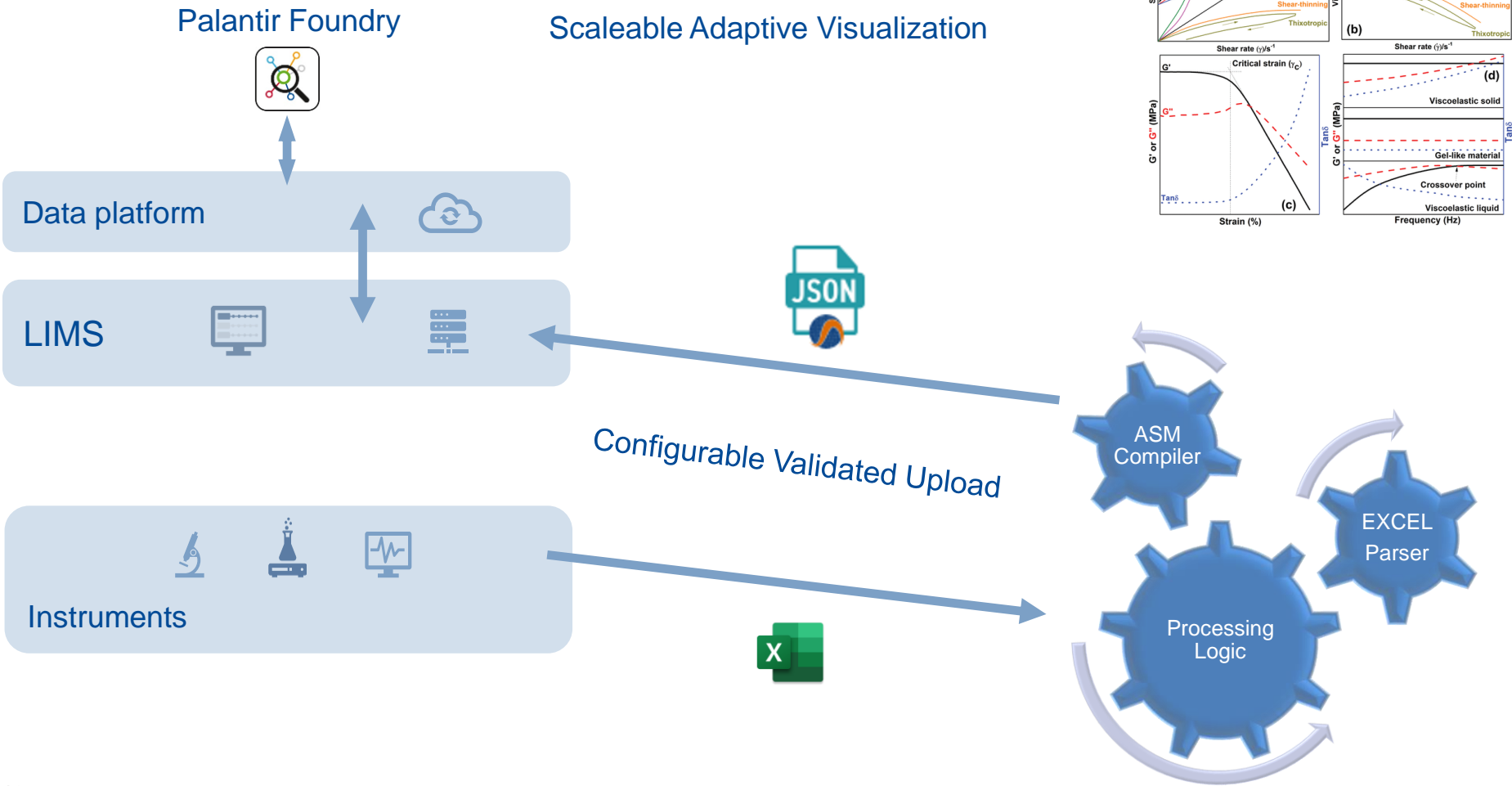
Clear Data Model
Intuitive Visualization

Data platform

LIMS

Configurable Validated Upload

ASM
Compiler

EXCEL
Parser

Processing
Logic

Instruments

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Instrument connection – The key to success …
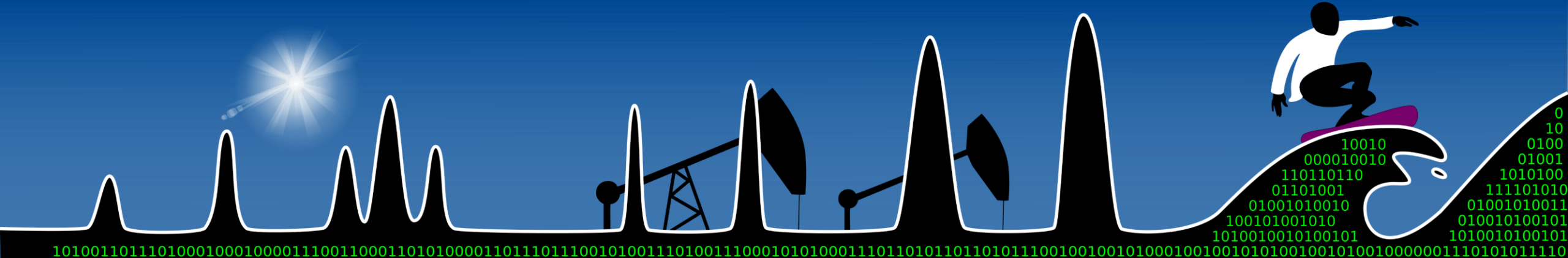
Standardization of interfaces in laboratories

A native support of

Standardized Communication Protocol (LADS/OPC-UA)
and
Standardized Data (File) Format (Allotrope)

by the data **producer** (instrument vendors) and data **consumer** (LIMS, ELN, … vendors)