



**BEST**  
PRACTICES  
AWARDS



**WINNER**

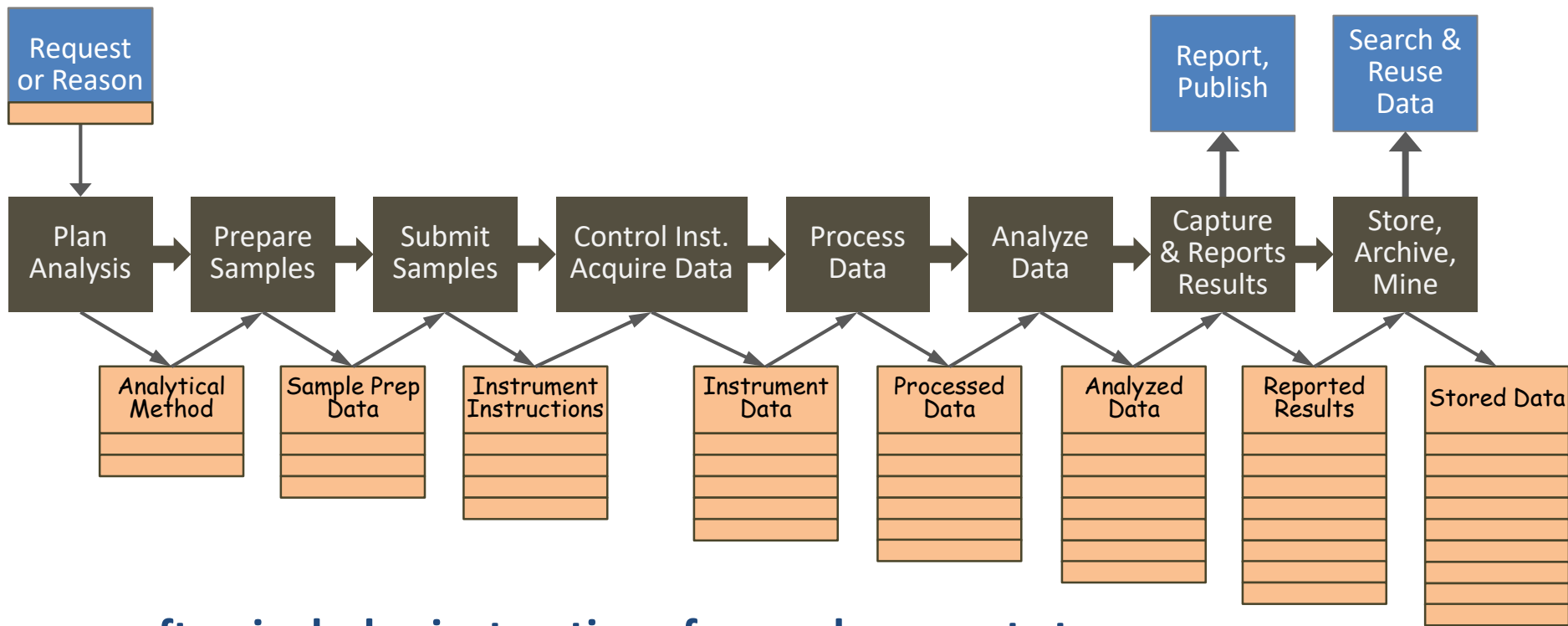
BioIT World 17  
CONFERENCE & EXPO

# Driving Outcomes Through Adoption of the Framework for Standardizing Data & Context

Allotrope Connect, April 9, 2019

Dassault Systemes, Vélizy-Villacoublay, France

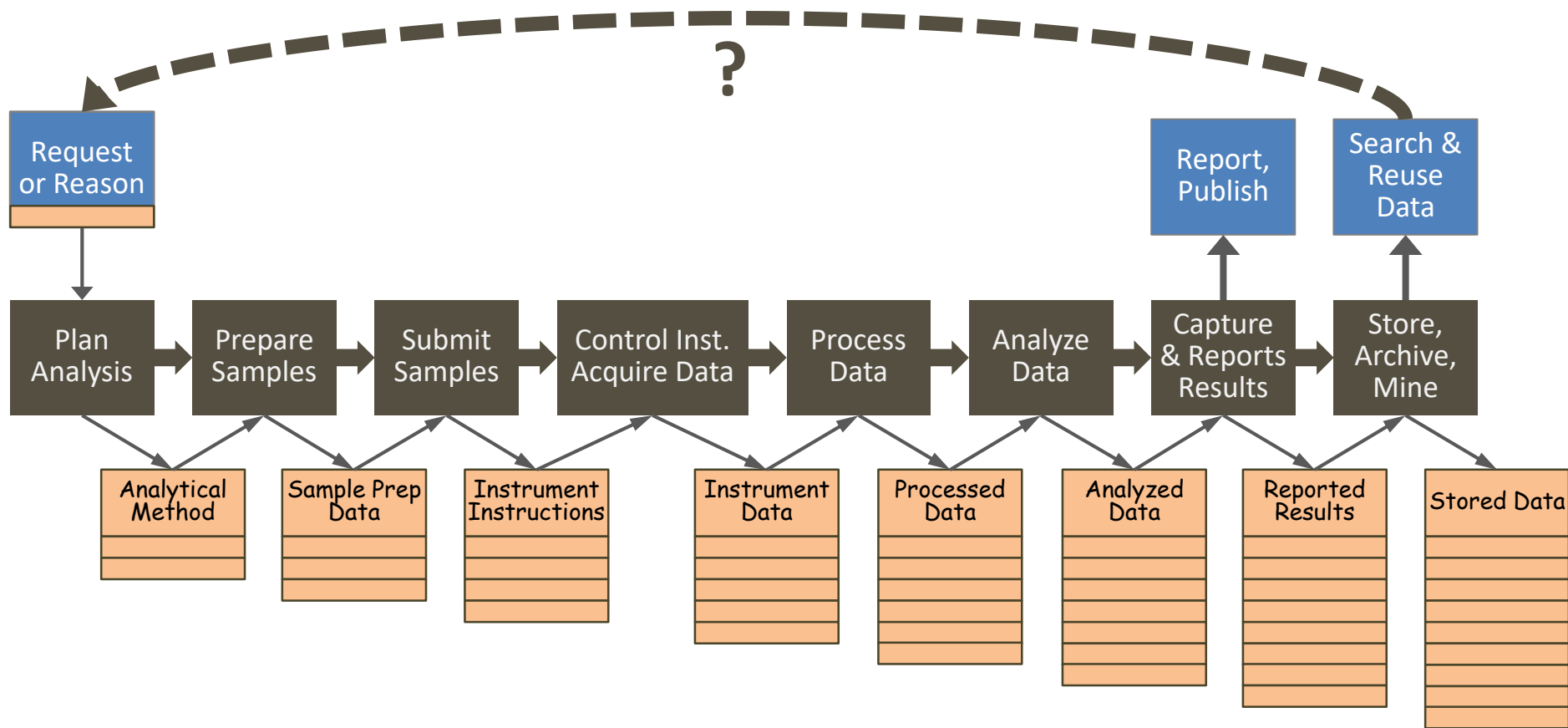
# Contextual meta data accumulates along every step of a workflow...



...often includes instructions for a subsequent step



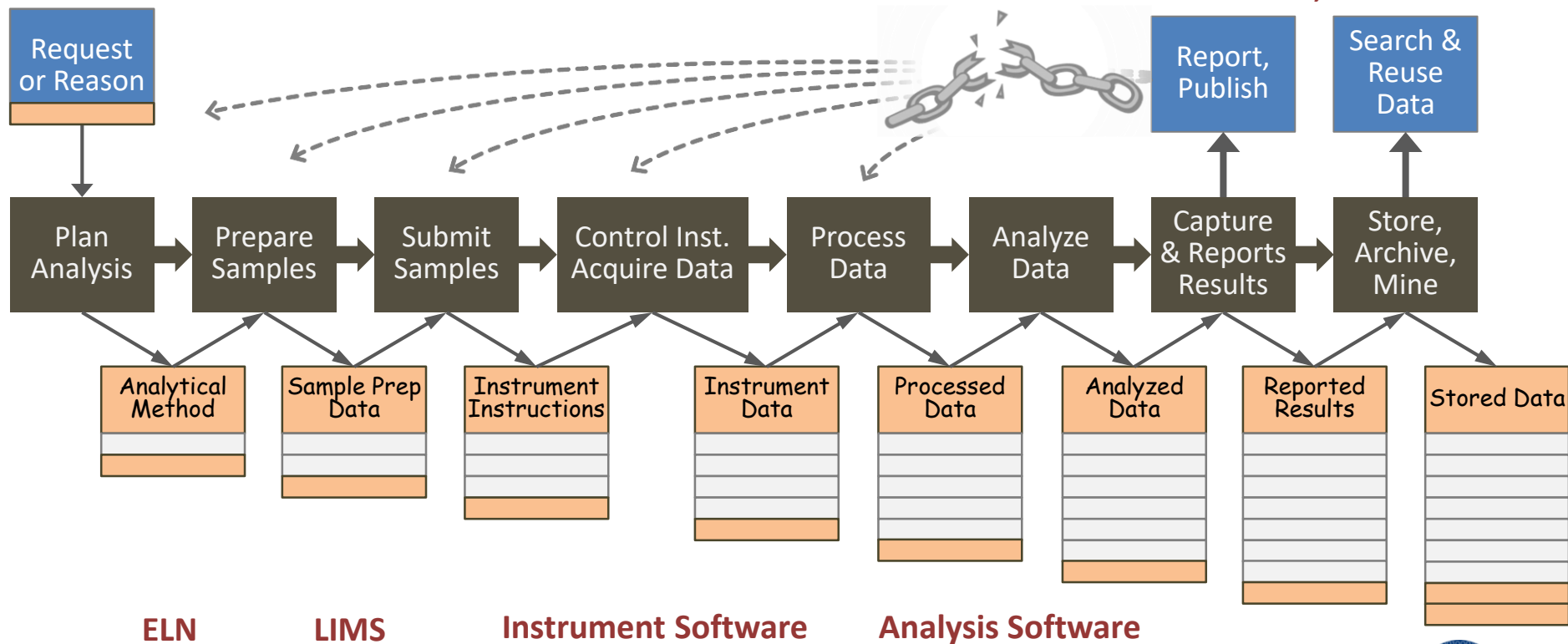
# Are we really leveraging our key asset??



# Contextual meta data accumulates along every step of a workflow... ... distributed in pieces across multiple systems & records

## Request 'System'

## File Shares, Databases



## Minimal interoperability

- a unique file format and data structure per app/system
- a bespoke or system specific API, custom integration, copy/paste
- Raw data & contextual information transfer *sometimes*, often just results

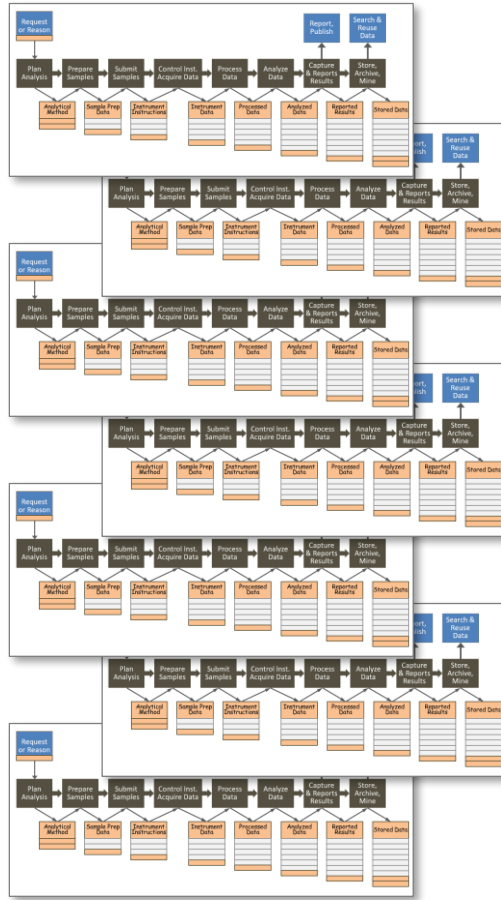
## Local languages and dialects

- Methods, parameters, etc. scattered across and transcribed between documents and/or applications
- Ambiguity in terminology
- Unstructured terms for metadata

## Context and meaning isolated from the data

- Meta data is not treated like a first class citizen
- A byproduct of process



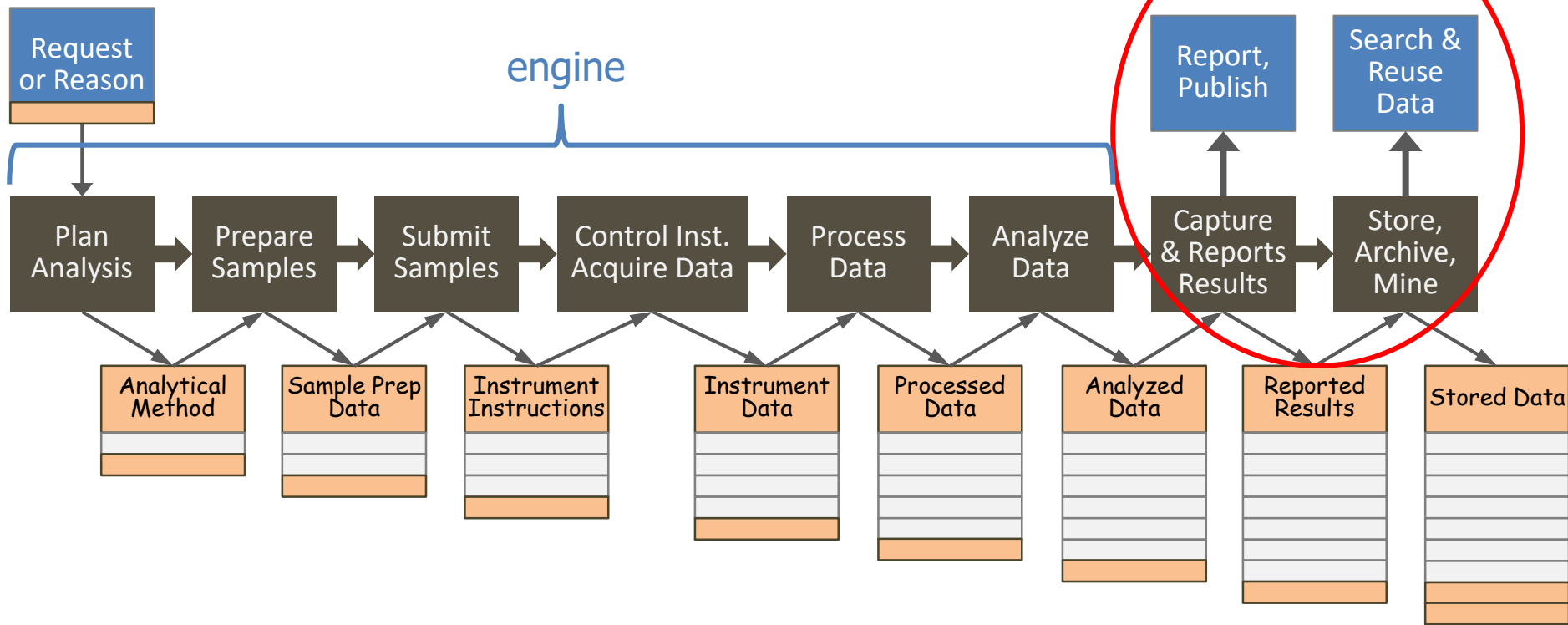


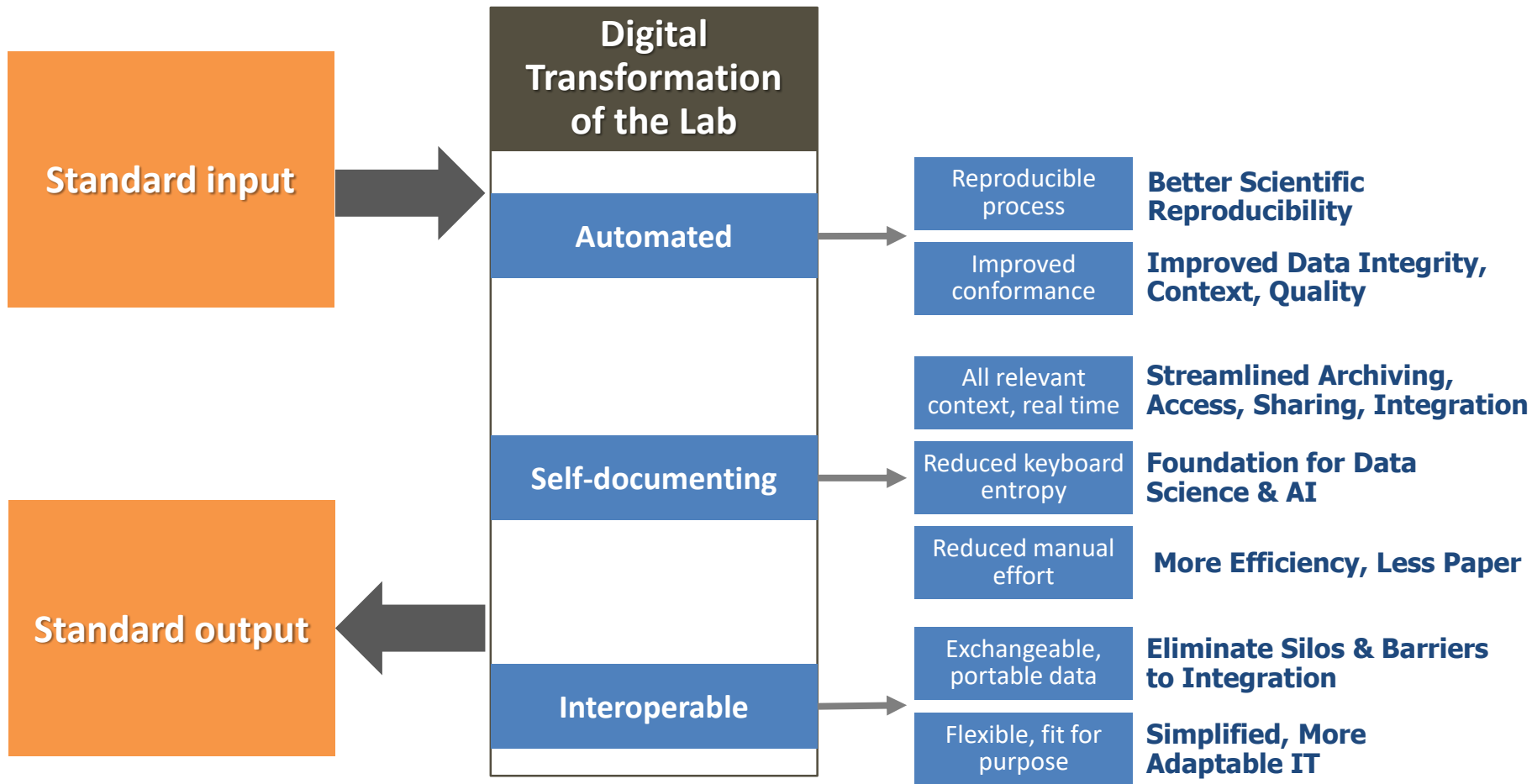
## Economies of scale?

- One study can encompass multiple measurements
  - Diverse: different measurements & instruments
  - Longitudinal: long term studies/time points
  - Distributed: groups, departments or companies
- Technology has never been moving faster than it is today



Yet, substantial effort in repair or clean-up is focused here.  
Limits quality & scale; no help to efficiency; automation opportunities?



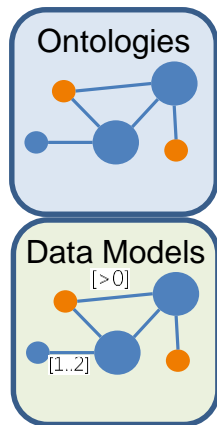




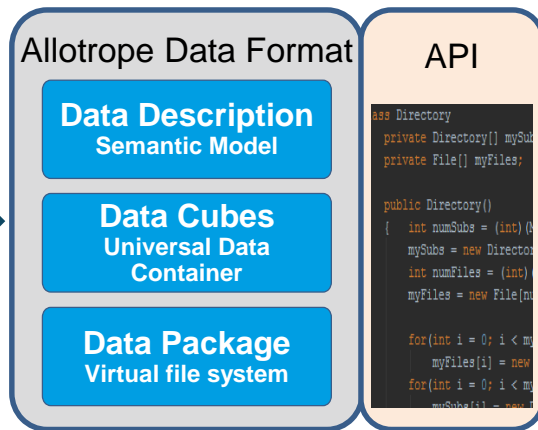
# The Allotrope Framework

A holistic approach in a modular extensible, architecture to enable the future state

Standard Vocabulary



Standard Data Structures

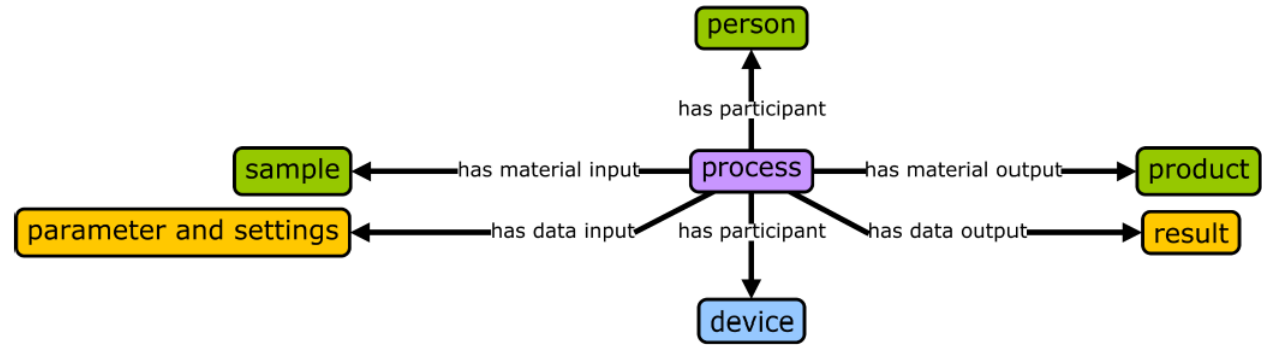
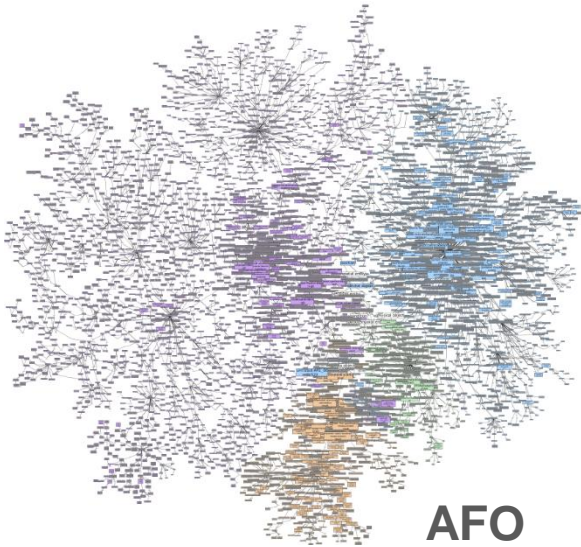
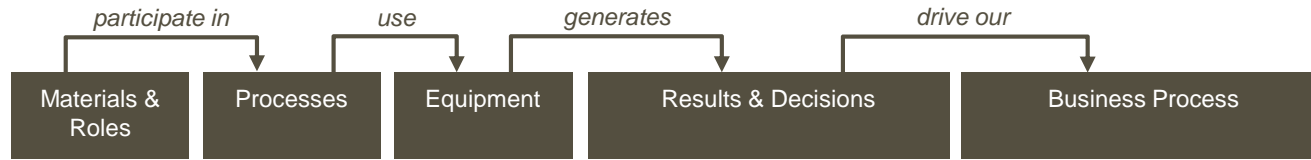


High-performance binary data format, instrument, technique, vendor agnostic

API for consistent implementation

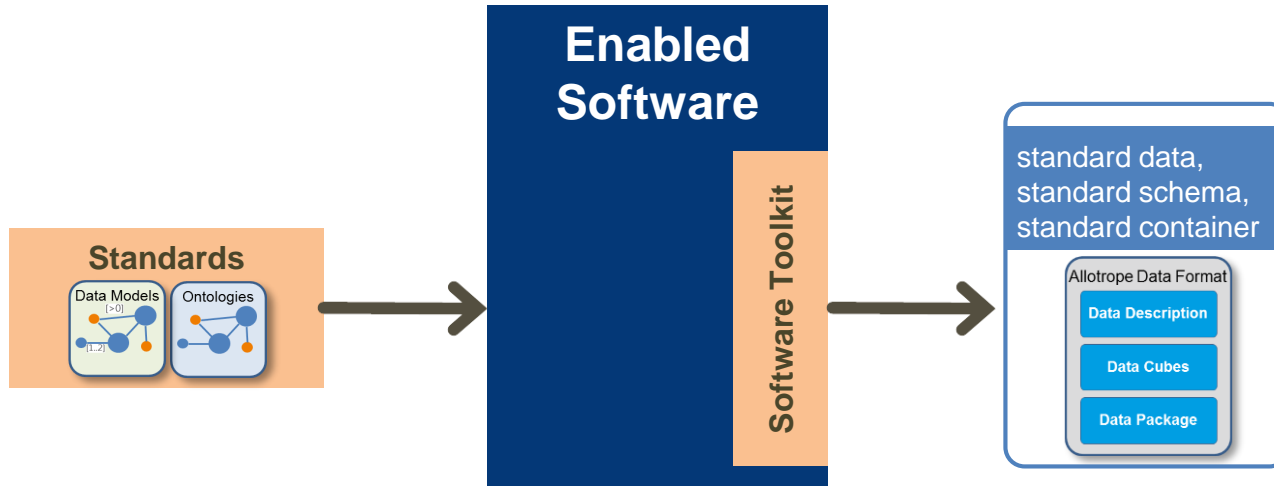
- Requirements defined by bio-pharma industry experts in application of instruments & data
- Result of extensive R&D on previous/existing standards
- The first format to integrate semantic standards & capabilities w/ raw data storage
- Ready to enable you to *revolutionize the way you acquire, share and gain insights from scientific data*



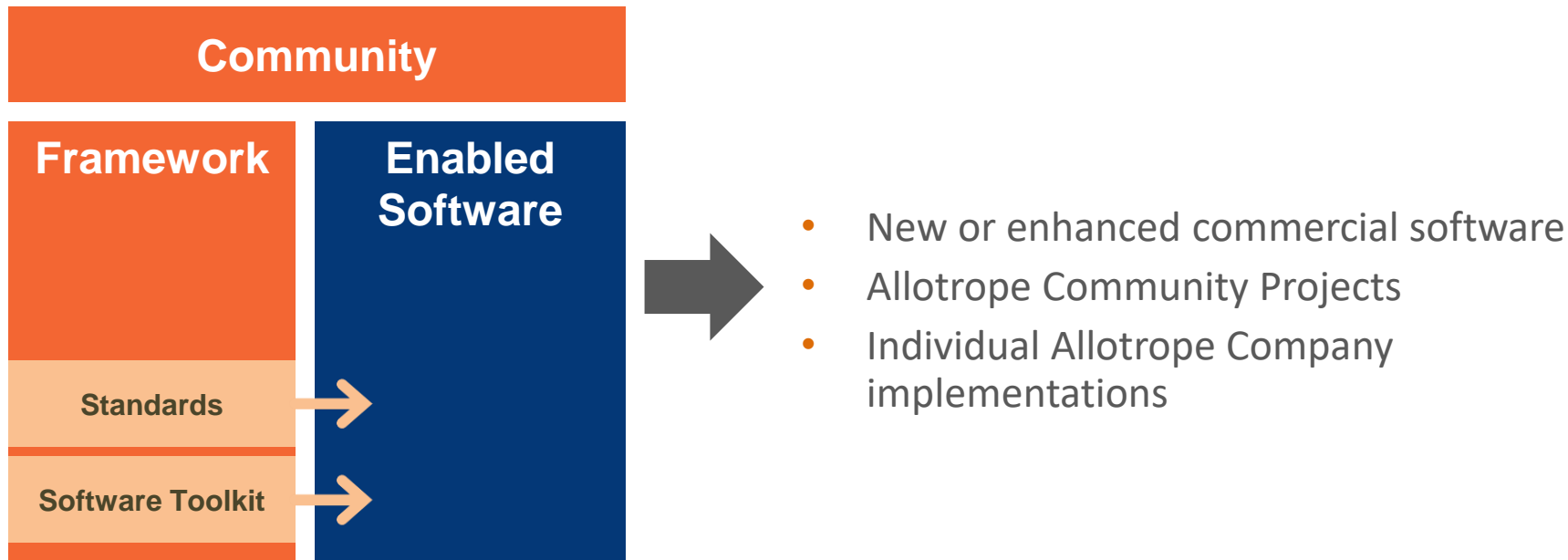


**AFO & ADM design & scope**

# Implementing the standards



# A community and the framework for standardization and linked data



# The Allotrope Community Today



abbvie

AMGEN

Baxter



OSTHUS  
success with R&D

AstraZeneca

Biogen

Boehringer  
Ingelheim



Bristol-Myers Squibb

Genentech  
A Member of the Roche Group



Lilly

MERCK  
INVENTING FOR LIFE

novo nordisk



Drinker Biddle



COGNITIVECHEM

The HDF Group

LABLICATION  
peak efficiency

Malvern  
Panalytical

L7INFORMATICS



TETRASCIENCE

Agilent Technologies

MESTRELAB RESEARCH  
Chemistry Software Solutions

SYNTHACE



Cognizant



PERSISTENT

SHIMADZU  
Excellence in Science



ZONTAL  
KNOWLEDGE CONNECTED



HALO  
DIGITAL

idbs

PerkinElmer  
For the Better

BIOVIA

Waters  
THE SCIENCE OF  
WHAT'S POSSIBLE.

ZIFO  
RnD SOLUTIONS

LAMSADE  
UMR CNRS 7243



sartorius

paradigm4

BIO-RAD

Cytobank

accenture

ELEMENTAL  
MACHINES

NPL

SCIEX



DEXSTR

BRUKER

University of  
Strathclyde  
Glasgow



ThermoFisher  
SCIENTIFIC



Riffyn

BSSN Software • Elemental Machines • Erasmus MC • Fraunhofer IPA • University of Michigan  
Mettler Toledo • NIST • Stanford University • University of Illinois at Chicago • University of Southampton



Allotrope Partner Network										Allotrope Member			
Informatics					Instrument					Pharma, Biopharma			
Abbott Informatics	BSSN Software	idbs	Mestrelab Research	Paradigm4	Agilent	GE Healthcare	Mettler Toledo	Sartorius	Abbvie	Amgen	AstraZeneca		
ACD/Labs	Cytobank	L7 Informatics	PerkinElmer	Synthace	Bio-Rad	LEAP Technologies	Sciex	ThermoFisher Scientific	Baxter	Bayer	Biogen		
Biovia	DEXSTR	Lablicate	Riffyn	ZONTAL	Bruker	Malvern	Shimadzu	Waters	Boehringer Ingelheim	Bristol-Myers Squibb	GSK		
Academic, Govt, non-profit					Services		IoT		Standards,...		Lilly	Novo Nordisk	Pfizer
					Accenture	Cognizant	Elemental Machines	Halo Digital	HDF Group				
					Persistent		Zifo RnD Solutions	TetraScience		National Institute of Standards and Technology (NIST)			
					Tata Consultancy Services			Analytics					
								Cambridge Semantics	CognitiveChem				



# The Allotrope Ecosystem

Public Repositories: OLS & BioPortal

Allotrope Repository

<https://allotrope.jfrog.io>

Allotrope PURL Server

<https://purl.allotrope.org>

Allotrope Documentation Server

<https://docs.allotrope.org>

...

Automated QC for Ontologies

Automation Infrastructure



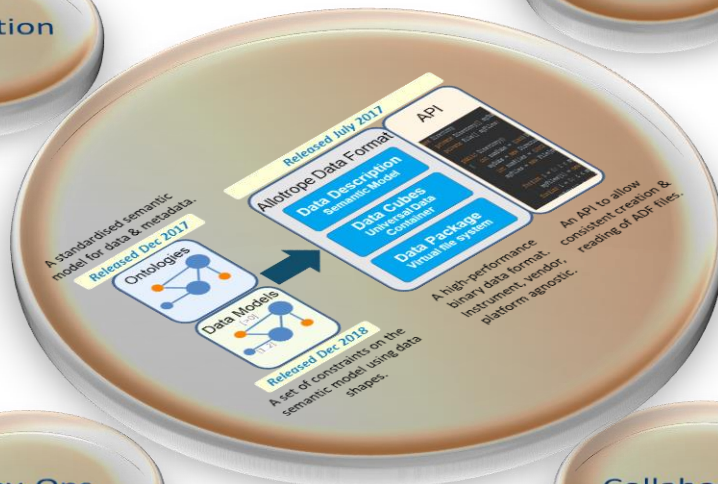
Data Viewers

Data Validators

Data Model Editors

QC Tools

...



Working Groups

Collaboration Infrastructure

18 Data Models in Progress



Pistoia:  
Method DB &  
Ontology Mapping



**Allotrope GitLab:** send email to 'allotrope-accounts@oisthus.com' for access.  
 Spring 2019 Allotrope Connect: week of April 8 hosted by Biovia in Vélizy-Villacoublay, France. Register [here](#). Check the [wiki](#) for updates.  
**ADF Explorer V1.1.5** now available. See [forum post](#) for more information.  
 LO-UV Data Model (V 2018.11) now available. See [forum post](#) for more information.  
**New AFO Release (V 2018.11)** now available. See [forum post](#) for more information.  
 Hotfix for C# ADF API v1.4.2 now available. See [forum post](#) for more information.

## Allotrope Foundation Collaboration Platform



### Important Dashboard Links:

<a href="#">Allotrope Main Contacts</a>	<a href="#">APN Member Main Contacts</a>	<a href="#">Group and Team Member Lists</a>
<a href="#">Decision Log</a>	<a href="#">Action Log</a>	<a href="#">Project Dashboard (definition)</a>
<a href="#">Allotrope Portfolio (files) (wiki)</a>	<a href="#">Issue Tracker (via GitLab)</a>	<a href="#">Proposed Work Request</a>

### Allotrope™ Software Downloads

<b>Allotrope™ Data Format APIs and Libraries</b> <ul style="list-style-type: none"> <li>Current (Release) Version (CSharp) (Java)</li> <li>Older (Release) Versions (CSharp) (Java)</li> <li>Release Candidate Versions (CSharp) (Java)</li> <li>Issue Tracker (via GitLab)</li> </ul>	<b>Allotrope Foundation<sup>2</sup> Ontologies</b> <ul style="list-style-type: none"> <li>Current (Release) Version</li> <li>Older (Release) Versions</li> <li>Release Candidate Versions</li> <li>Issue Tracker (via GitLab)</li> </ul>	<b>Allotrope™ Data Models</b> <ul style="list-style-type: none"> <li>Current (Release) Version</li> <li>Older (Release) Versions</li> <li>Release Candidate Versions</li> <li>Issue Tracker (via GitLab)</li> </ul>
	<b>Allotrope™ Data Format Explorer (ADF Explorer)</b> <ul style="list-style-type: none"> <li>Current (Release) Version</li> <li>Older (Release) Versions</li> <li>Release Candidate Versions</li> <li>Issue Tracker (via GitLab)</li> </ul>	

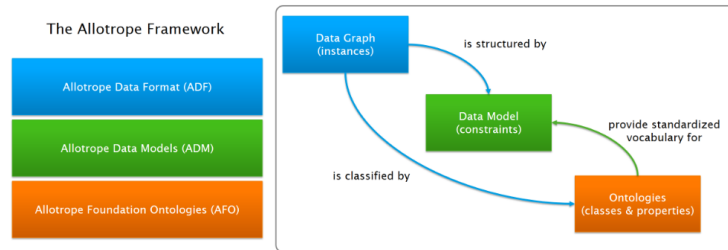
### Important Resources Links:

<b>Marketing Materials</b> <ul style="list-style-type: none"> <li>Allotrope Logos (AF Member Use)</li> <li>APN Logos</li> </ul>	<b>Contributed Software</b>	<b>Allotrope™ Training Materials</b>
<b>Allotrope™ Connect Workshop Materials: Apr 2019</b>	<b>Allotrope™ Town Hall Materials:</b>	<b>External Resources</b>



The Allotrope Framework is composed of the following core components: the Allotrope Data Format (ADF), the Allotrope Data Models (ADM), and the Allotrope Foundation Ontologies (AFO). The ADF stores data graph instances that are structured according to the ADM and classified according to the AFO. The ontologies provide standardized vocabularies for the data model constraints.

### The Allotrope Framework



#### Allotrope Data Format (ADF)

The ADF is a family of specifications designed to standardize the acquisition, exchange, storage and access of analytical data captured in laboratory workflows. It is intended for the long-term stability of archived analytical data and fast real-time access.

#### Allotrope Data Models (ADM)

The ADM constrains how ontologies are used using the Shapes Constraint Language (SHACL) expressed as RDF triples. SHACL allows the definition of data structures (e.g. schemas, templates) that describe how to use ontologies in a standardized (i.e., reproducible, predictable, and verifiable) manner.

#### Allotrope Foundation Ontologies (AFO)

The AFO is an ontology suite that provides a standard vocabulary and semantic model for the representation of laboratory analytical processes. The AFO suite is aligned at the upper layer to the Basic Formal Ontology (BFO). The core domains modeled include: Equipment, Material, Process, and Results.

The current list of technical reports for the above products are itemized below by category:

- Allotrope Data Format Overview
- ADF API Specifications
  - ADF Data Package API
  - ADF Data Cube API
  - ADF Data Description API
  - ADF Data Store API
  - Audit Trail and Electronic Signature Specification
  - ADF Checksums
- Ontology and Taxonomy Specifications
  - ADF Data Package Ontology
  - ADF Data Cube Ontology
  - ADF Data Cube to HDF5 Mapping Ontology
- Reference Documentation
  - Allotrope ADF Java Doc (APIs)
  - CWL Docs (Ontologies & Taxonomies)
- Developer's Guides
  - Data Package
  - Data Cube
  - Data Description
- Reference Documentation
  - Ontologies & Taxonomies

Available [releases](#) by date.







Projects



New project

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All   Personal

-  Allotrope / **afo**  Developer  
Allotrope Foundation Ontologies  



★ 0   🔍 0   📄 1   📦 38   ⚠️

Updated 6 hours ago
-  Allotrope Open Source / **allotrope-devops**  Developer  
Documentation of the DevOps procedures  



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Updated 6 hours ago
-  Allotrope / **adf**  Developer  
The Allotrope Data Format  



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Updated 13 hours ago
-  Allotrope Open Source / **adf-primer-java**  Developer  



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Updated 4 days ago
-  Allotrope Open Source / **ontology-qa-tools**  Developer  
Allotrope Ontology QA Tools  



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Updated 4 days ago
-  Allotrope Community Projects / **ChromatographyWG-SQD-MS**  Developer  
The ChromatographyWG SQD-MS Data Model  

★ 0   🔍 0   📄 0   📦 6

Updated 5 days ago
-  Allotrope Community Projects / **allotrope-lcms-datamodel**  Developer  
LC-MS model  

★ 1   🔍 0   📄 0   📦 0

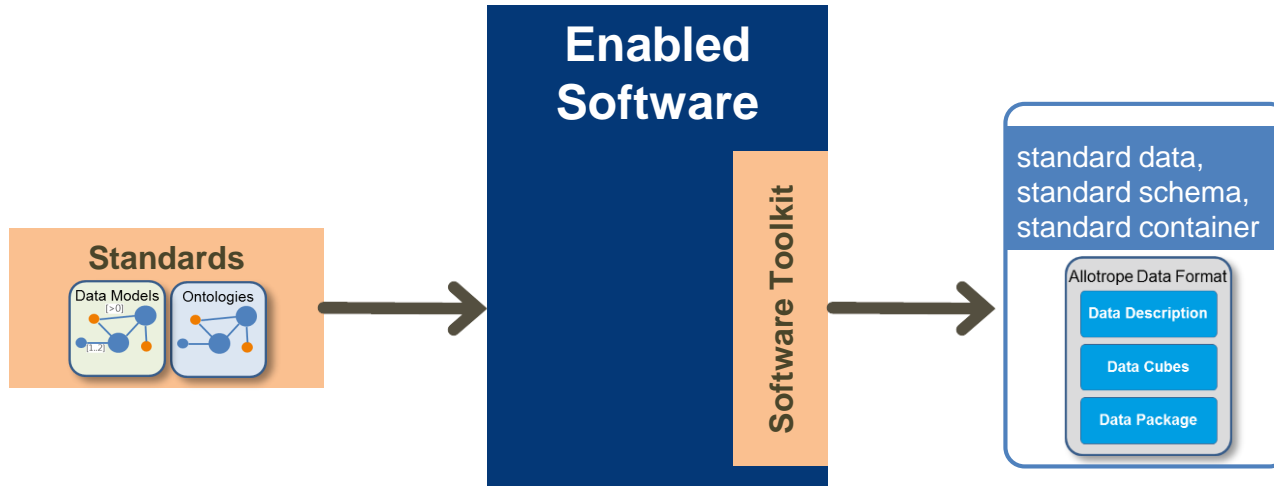
Updated 6 days ago
-  Allotrope Community Projects / **merck-column**  Developer  
The Merck Column Model  

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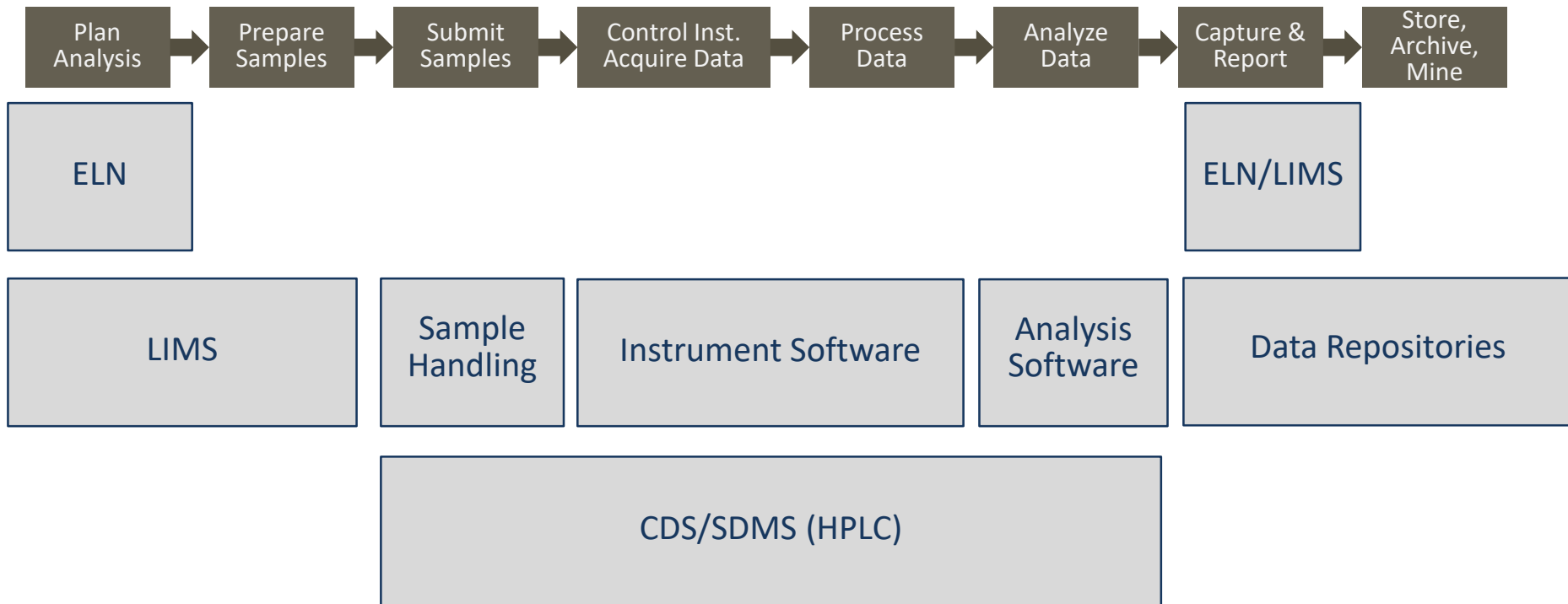
Updated 1 week ago



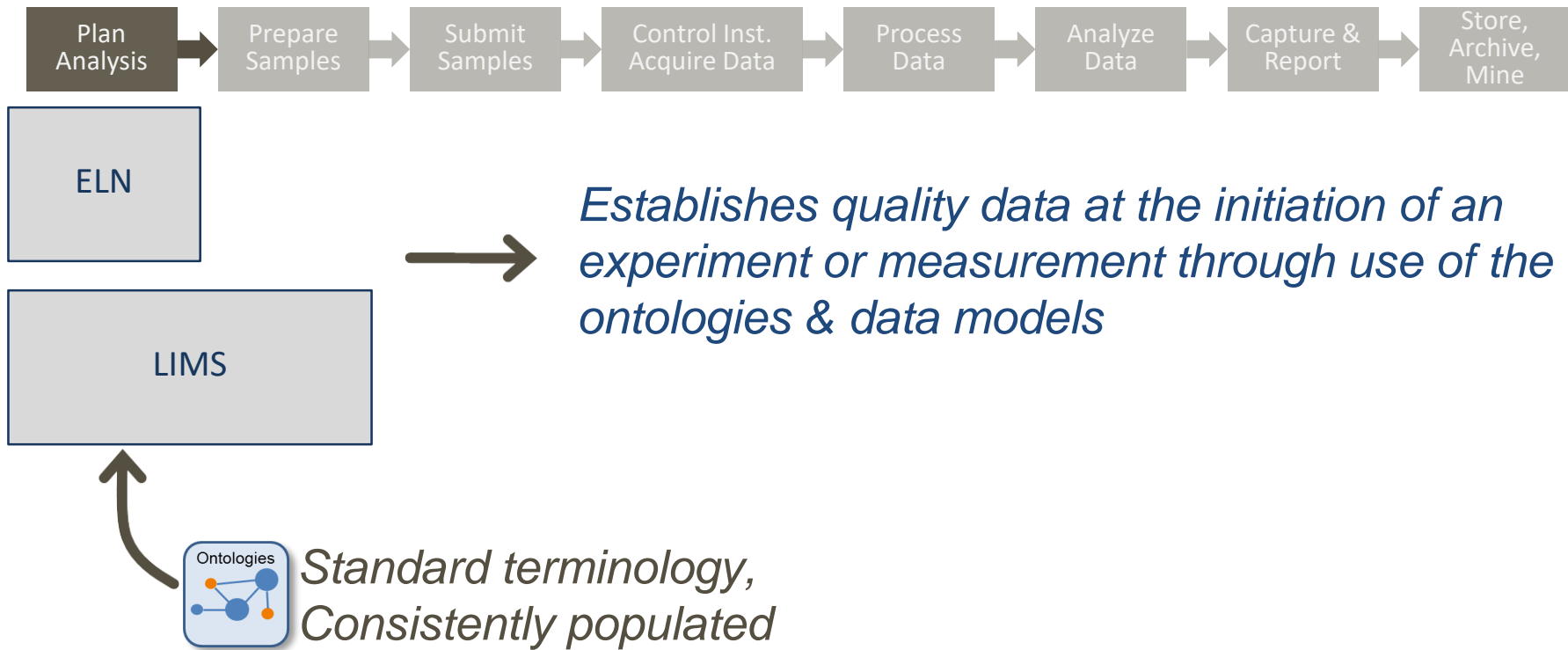
# Implementing the standards



# Examples of integrating the standards with typical informatics capabilities



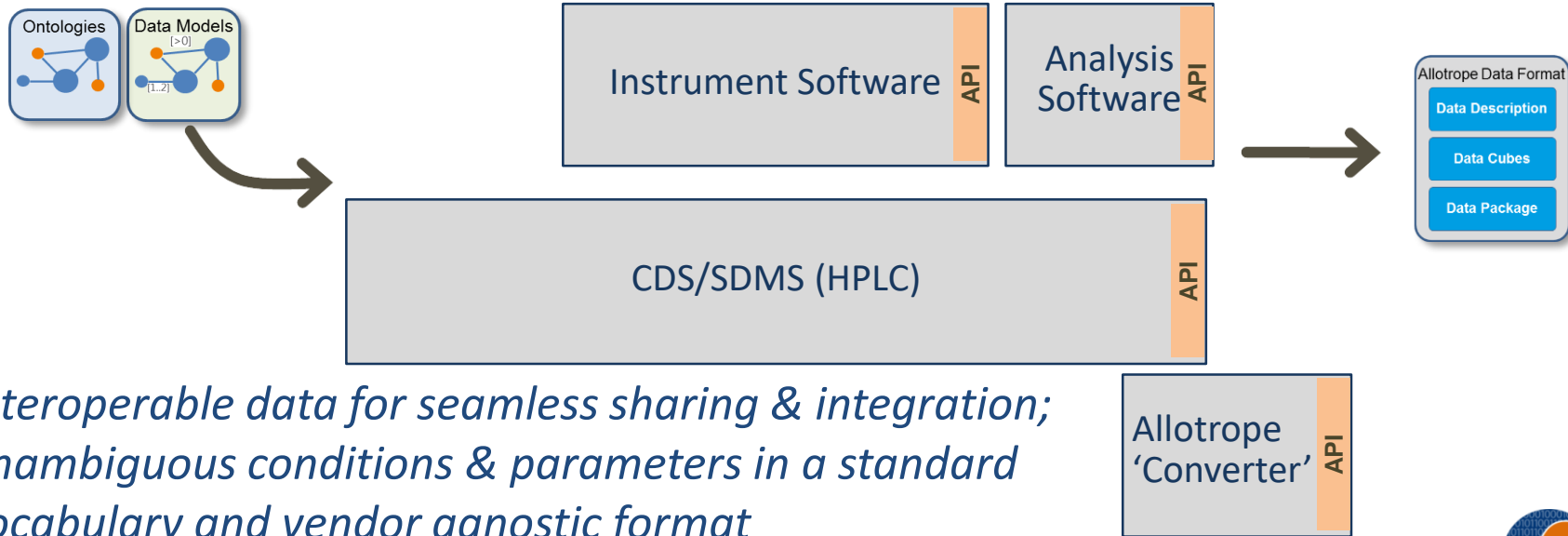
# Examples of integrating the standards with typical informatics capabilities



# Examples of integrating the standards with typical informatics capabilities



*Standard terminology  
& data models*



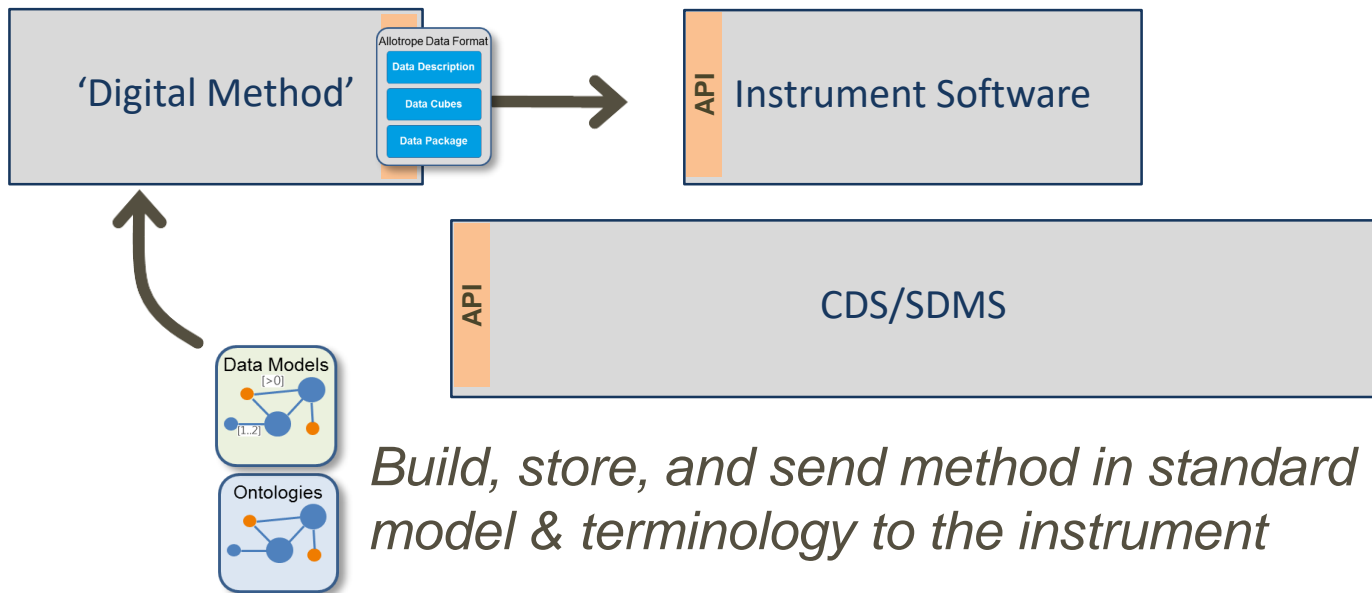
*Interoperable data for seamless sharing & integration;  
unambiguous conditions & parameters in a standard  
vocabulary and vendor agnostic format*



# Examples of integrating the standards with typical informatics capabilities



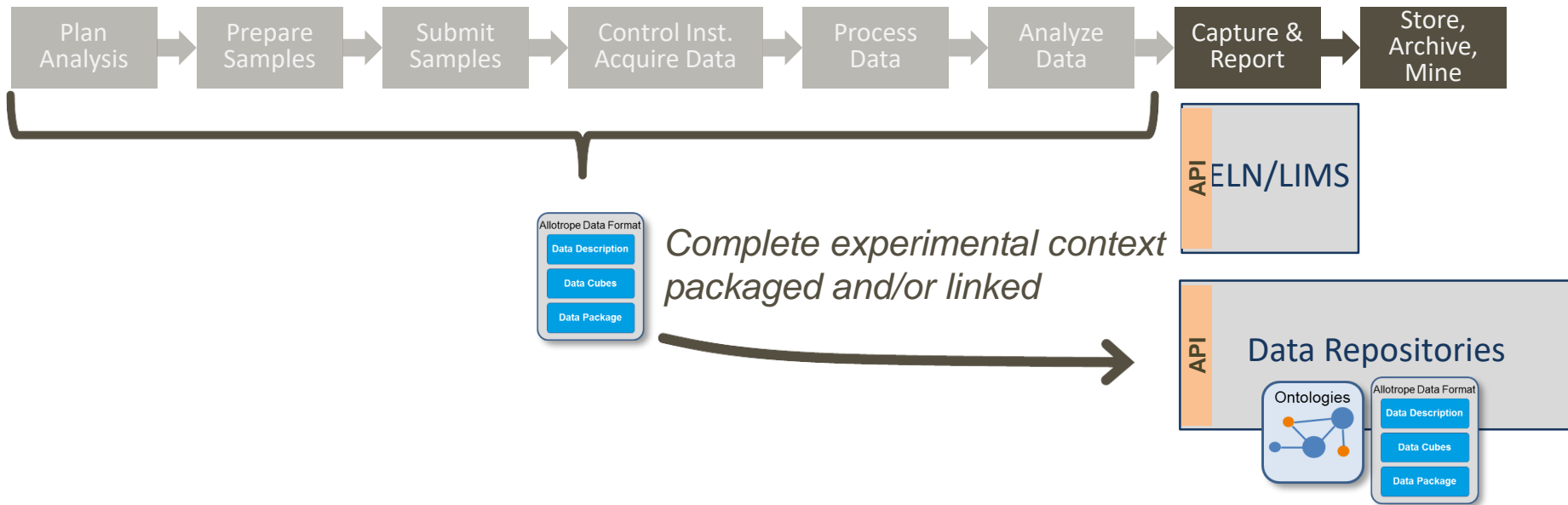
*New opportunity to reduce manual effort to improve efficiency AND reproducibility*



*Build, store, and send method in standard data model & terminology to the instrument*



# Examples of integrating the standards with typical informatics capabilities

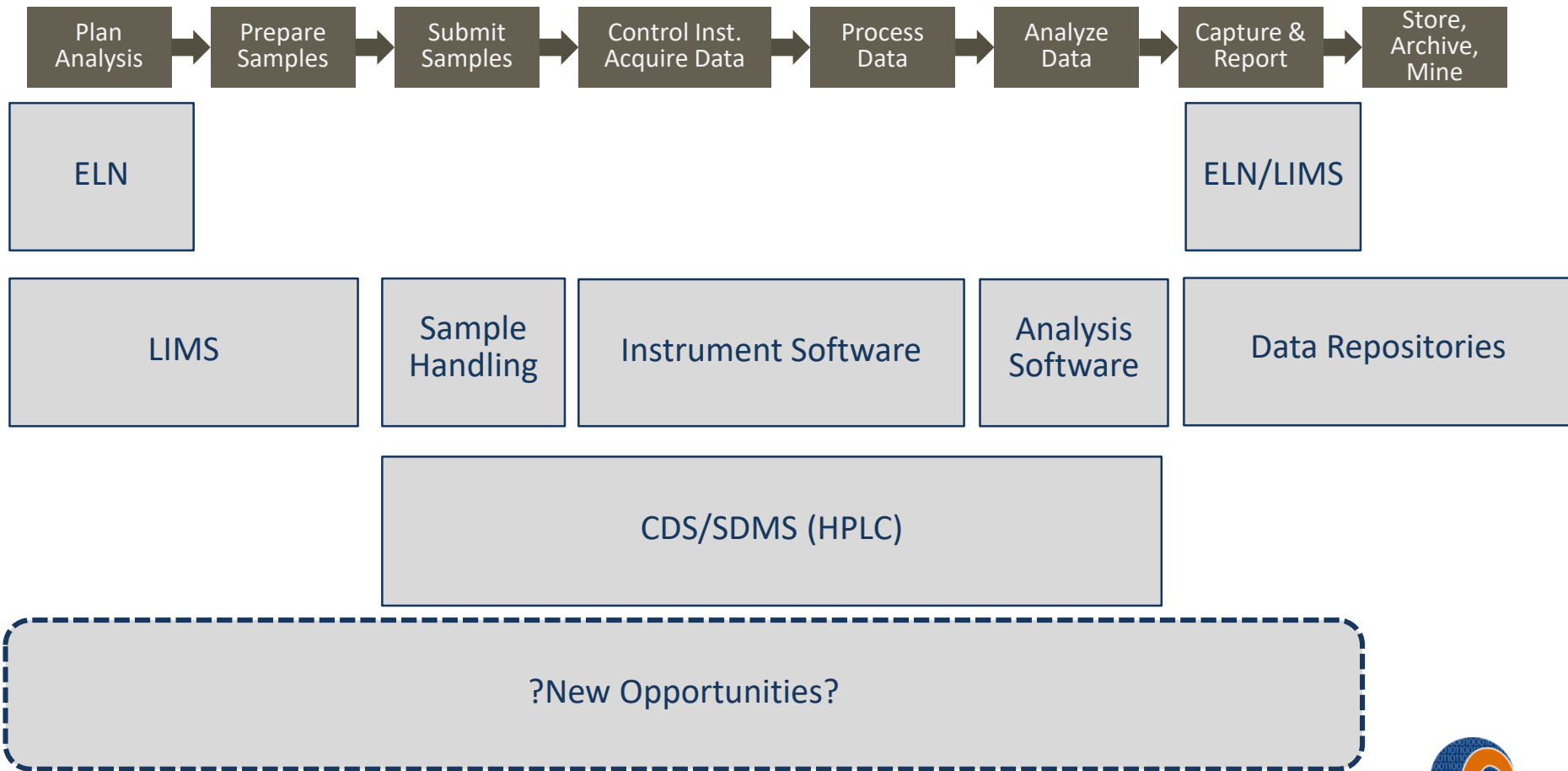


*Data is reusable & interoperable; future proof from obsolescence.*

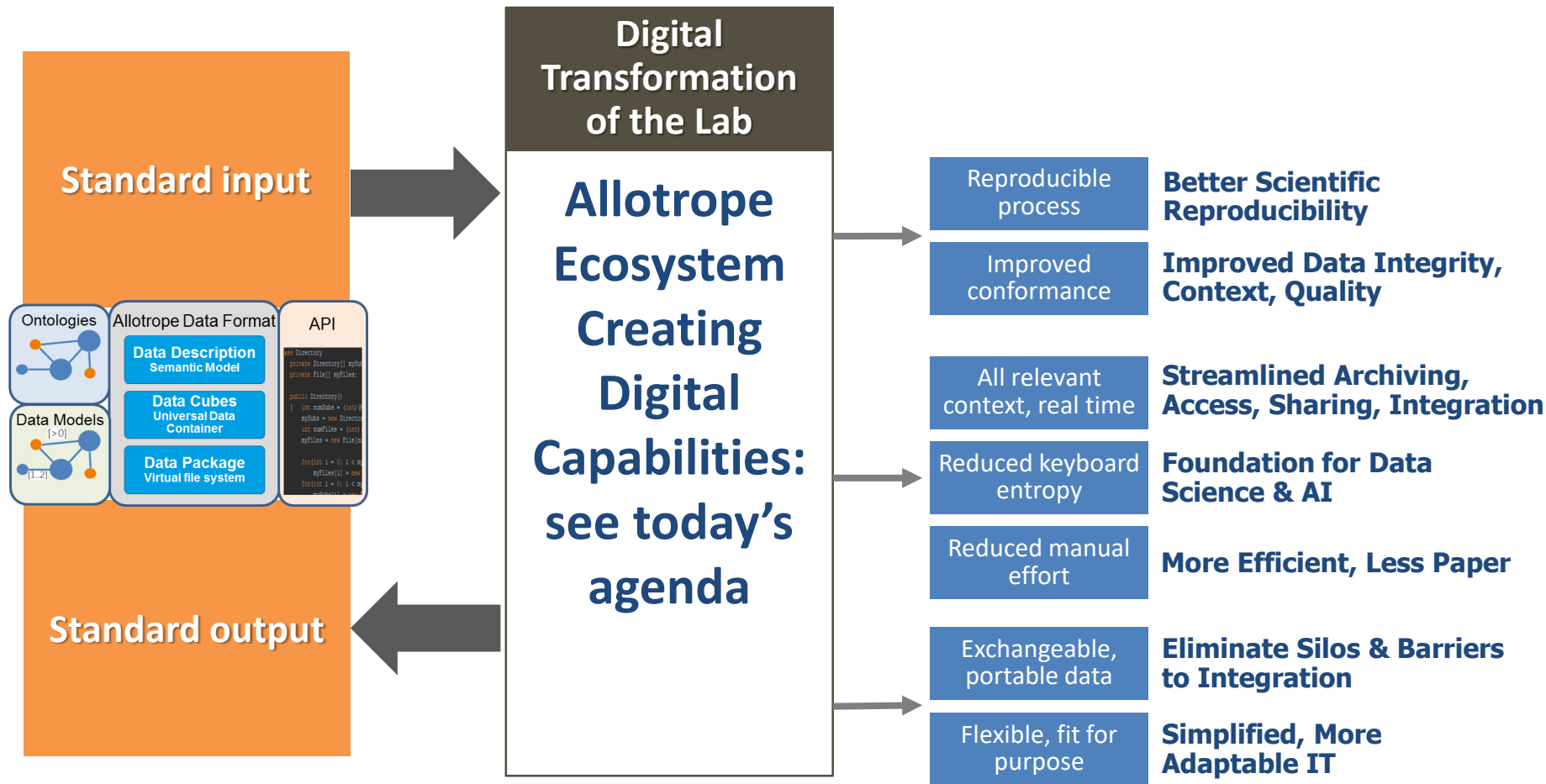
*Why just search when you can find? The annotation is complete & consistent across instrument, lab, group, department, or company?*



# Any of these can be a starting point for your transformation...







# Thank you!

**Fall 2019 Allotrope Connect October 7-11, 2019**

Hosted by Genentech in San Francisco, CA.

For more info, please contact the Secretariat at [more.info@allotrope.org](mailto:more.info@allotrope.org) or [dana.vanderwall@bms.com](mailto:dana.vanderwall@bms.com)

[www.allotrope.org](http://www.allotrope.org)

