



Welcome to Allotrope Connect Spring 2023



We are a consortium of chemical & life sciences companies, instrument & software vendors, and academic & government institutions formed from IQ Consortium in 2013.

We revolutionize the way we acquire, share and gain insights from scientific data through application of community-derived data standards consistently delivered via an extensible technology framework.



New Paradigm: Data-Centric Environment

- Data are a key asset of any organization
- Data are self-describing and do not rely on an application for interpretation & meaning
- Data are expressed in open, non-proprietary formats
- Access to and security of the data is a responsibility of the data layer, and not managed by applications
- Applications are allowed to visit the data, perform their magic and express the results of their process back into the data layer for all to share



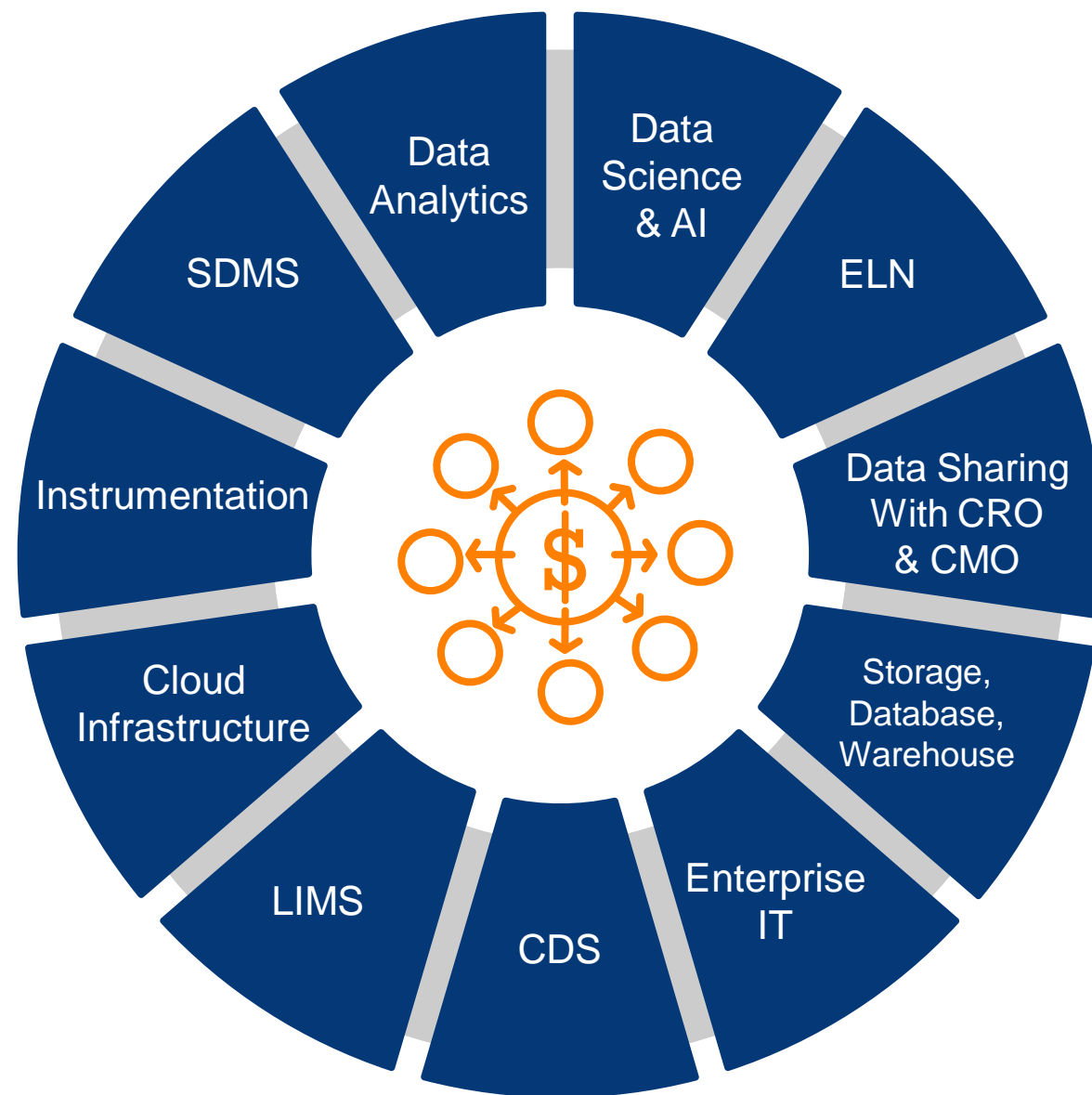
<http://www.datacentricmanifesto.org>



Impact of R&D Current State on IT

The high cost of being application-centric

- Custom integrations
- Endless relational data mappings
- Lack of modularity
- Technology incompatibilities
- Vendor lock-in with proprietary formats
- Custom data analysis tools
- Complex data sharing
- Complex data migrations
- Wasting valuable resources
- Less bandwidth to drive modeling & data science



Data Standardization Creates FAIR Data

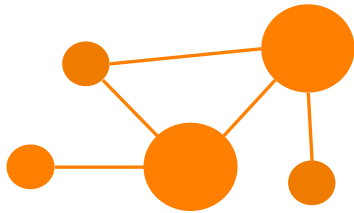
- ✓ FAIR provides principles, data standards provide the blueprint for a solution
- ✓ Defines data quality goals across all solutions
 - **Context**
 - **Structure**
 - **Format**
- ✓ Can standardize anywhere in data lifecycle, but is foundational if done at data capture
- ✓ Standardization across domains creates data interoperability and ease of (re)use by design



Data standards help build a strong data foundation, brick by brick.



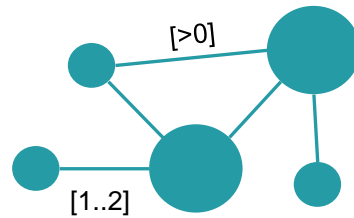
Allotrope Framework Products



AFO

Allotrope Foundation
Ontologies

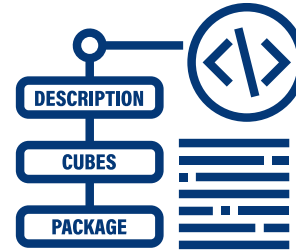
Defines terms & their
relationships consistently
across laboratory domains



ADM

Allotrope Data
Models

Establishes schema for
consistent use of ontologies to
describe laboratory items



ADF

Allotrope Data
Format

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

{a:1}
{b:2}

ASM

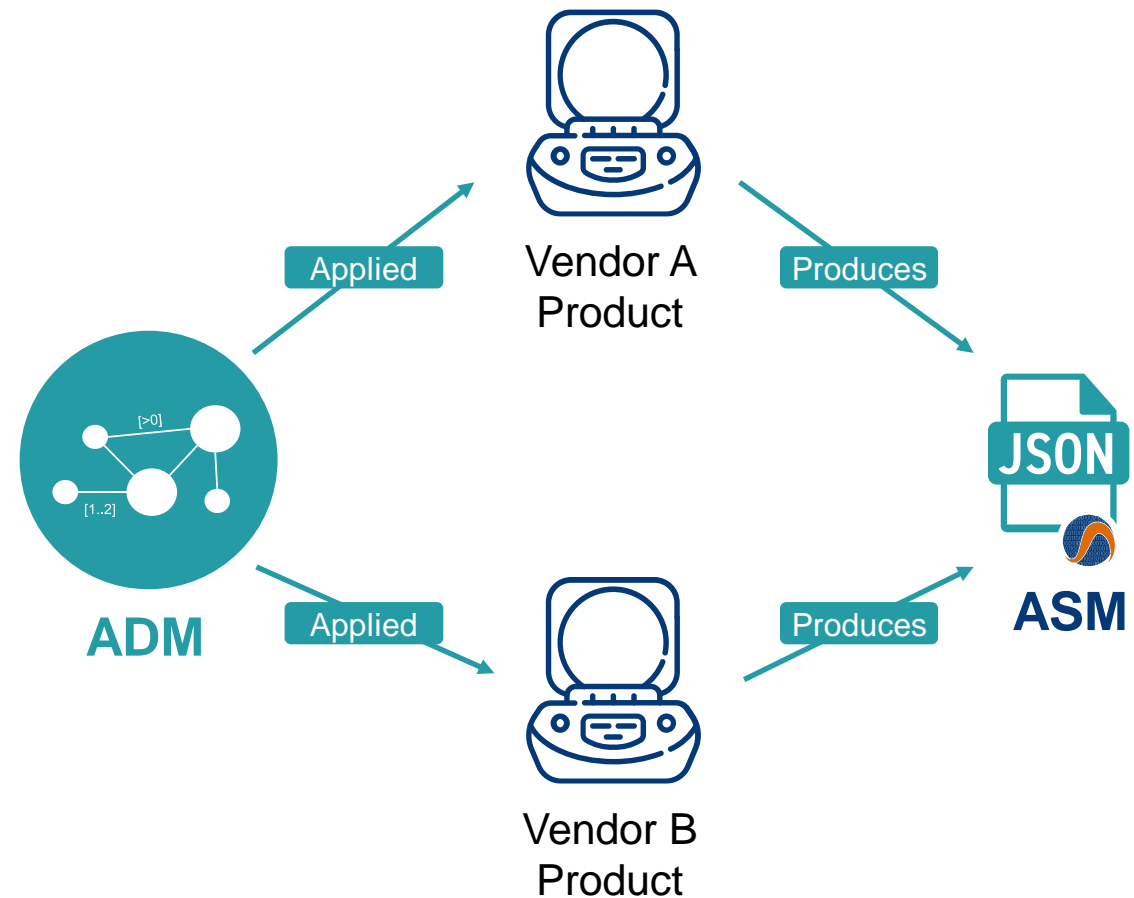
Allotrope Simple
Models

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



Allotrope Data Models (ADM)

- Scope determined by what information is needed within a use case(s)
- Leverages terms and relationships found in Allotrope Foundation Ontologies (AFO)
- Provides a schema to consistently structure data to describe something in the lab (e.g., an instrument or result)
- Simplest application is to create an **Allotrope Simple Model (ASM)** via automation



The Allotrope Catalog Today

57 domain models available today as ADM and/or ASM

- Automated Reactors / PAT
- Dissolution
- **Liquid Chromatography***
- Oven/Coulometric KF
- Specific Rotation
- Balance
- Blood Gas Analyzer
- Electrochemical Tester
- Liquid Particle Counter
- **pH Sensor***
- LC-MS
- Osmolality
- Surface Area Analysis
- Bulk Density
- **FPLC***
- Live-cell imaging
- qNMR
- **Hot Tack***
- **Temperature Monitoring***
- Calibration
- FTIR
- Loss on Drying (Moisture Analysis)
- qPCR
- Cell Counting
- **Fluorescence***
- **Luminescence***
- Raman
- **UV Absorbance***
- **Gas Chromatography***
- Methods: LC-UV
- Water Activity Tester
- Conductivity
- Hardness Tester
- Nephelometry
- **Foam Height***
- **Foam Qualification***
- **Stirring***
- Titration (inclusive of KF)
- X-Ray Powder Diffraction
- Differential Scanning Calorimetry (DSC)
- High Resolution MS
- Optical Microscopy
- Single Quad-Mass Spec(SQD-MS)
- Disintegration
- **Pumping***
- Sample Preparation Process Workflow
- Light Obscuration (Liquid Particle Counter)
- Cell Culture Analyzer (Metabolite Analyzer)
- Size Exclusion Chromatography
- Dynamic Vapor Sorption Analyzer
- Particle Size Distribution (PSD)
- Supercritical Fluid Chromatography
- Scanning Electron Microscope (SEM)
- Thermogravimetric Analysis
- **Pressure Monitoring***
- **Tensile Testing***

**New or Updated in last 6 months*

...and more added each quarter! Allotrope Data Models (ADM)



Allotrope Foundation Ontologies (AFO)

- Allotrope Foundation Taxonomies (AFT) define and classify terms into five domains
- Allotrope Foundation Ontologies (AFO) link terms across domains for deeper context
- AFO assigns unique identifiers to terms so software can unambiguously track their use
- AFO is conveniently available through your web browser at the [Public Bioportal Link](#)
- Can be used to enrich existing data sets



New!

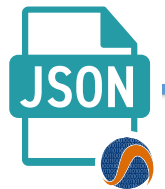
Available on OLS, Ontobee, and as a Thesaurus



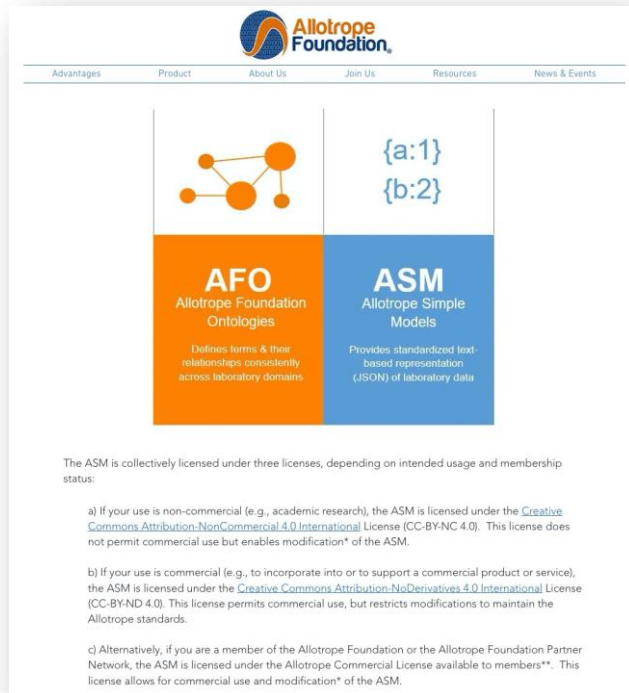
Allotrope Simple Models (ASM)

- Bidirectionally compatible with the corresponding Allotrope Data Model (ADM)
- Leverages JSON, a preferred data format of data scientists, that works with any programming language and has many publically-available software tools to support its use
- Both human and machine readable
- Easy to directly apply to use cases where simple data structures are sufficient (e.g., associate parameter with result)

```
{"$comment": "Conductivity ASM",
"$asm.manifest": "http://purl.allotrope.org/adm/manifest/pcr/CR/2021/09/conductivity.manifest",
"measurement identifier": "413befdd",
"measurement time": "2015-09-24T03:47:13.001Z",
"analyst": "Amgentoaks1",
"sample identifier": "unknown-10",
"equipment serial number": "278882456",
"batch identifier": "XYZ",
"conductivity": {
  "value": 273000,
  "unit": "S/m"
},
"temperature": {
  "value": 28.6,
  "unit": "degC"
}
}
```



Allotrope Simple Models are open to all!



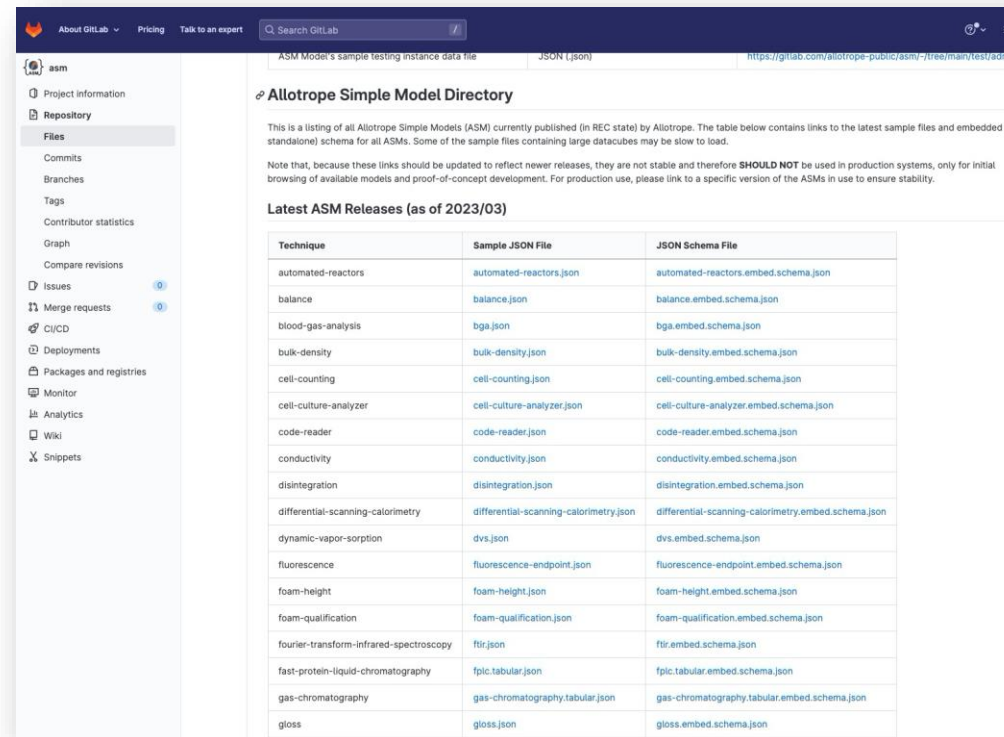
The image shows a screenshot of the Allotrope Foundation website. At the top, there is a navigation bar with links for Advantages, Product, About Us, Join Us, Resources, and News & Events. Below this, there are two main sections: AFO (Allotrope Foundation Ontologies) and ASM (Allotrope Simple Models). The AFO section is highlighted in orange and describes defining terms and relationships consistently across laboratory domains. The ASM section is highlighted in blue and describes providing standardized text-based representation (JSON) of laboratory data. Below these sections, there is a paragraph about the licensing of ASM and three numbered points (a, b, c) detailing the license conditions for non-commercial, commercial, and member use.

AFO
Allotrope Foundation Ontologies
Defines terms & their relationships consistently across laboratory domains.

ASM
Allotrope Simple Models
Provides standardized text-based representation (JSON) of laboratory data.

The ASM is collectively licensed under three licenses, depending on intended usage and membership status:

- If your use is non-commercial (e.g., academic research), the ASM is licensed under the [Creative Commons Attribution-NonCommercial 4.0 International License](#) (CC-BY-NC 4.0). This license does not permit commercial use but enables modification* of the ASM.
- If your use is commercial (e.g., to incorporate into or to support a commercial product or service), the ASM is licensed under the [Creative Commons Attribution-NoDerivatives 4.0 International License](#) (CC-BY-ND 4.0). This license permits commercial use, but restricts modifications to maintain the Allotrope standards.
- Alternatively, if you are a member of the Allotrope Foundation or the Allotrope Foundation Partner Network, the ASM is licensed under the Allotrope Commercial License available to members**. This license allows for commercial use and modification* of the ASM.



The image shows a screenshot of the Allotrope Simple Model Directory on GitHub. The page title is "Allotrope Simple Model Directory". Below the title, there is a note stating that the table contains links to the latest sample files and embedded JSON schema for all ASMs, and that some files may be slow to load. A warning note indicates that the links should be updated to reflect newer releases and that they should not be used in production systems. Below the note, there is a section titled "Latest ASM Releases (as of 2023/03)" which contains a table with three columns: Technique, Sample JSON File, and JSON Schema File. The table lists various techniques and their corresponding files.

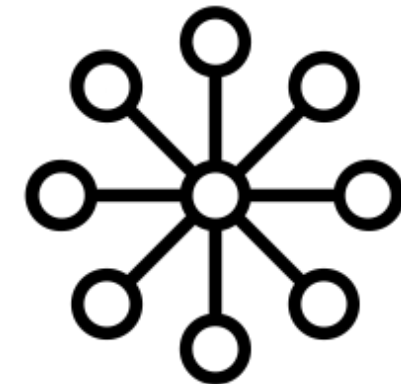
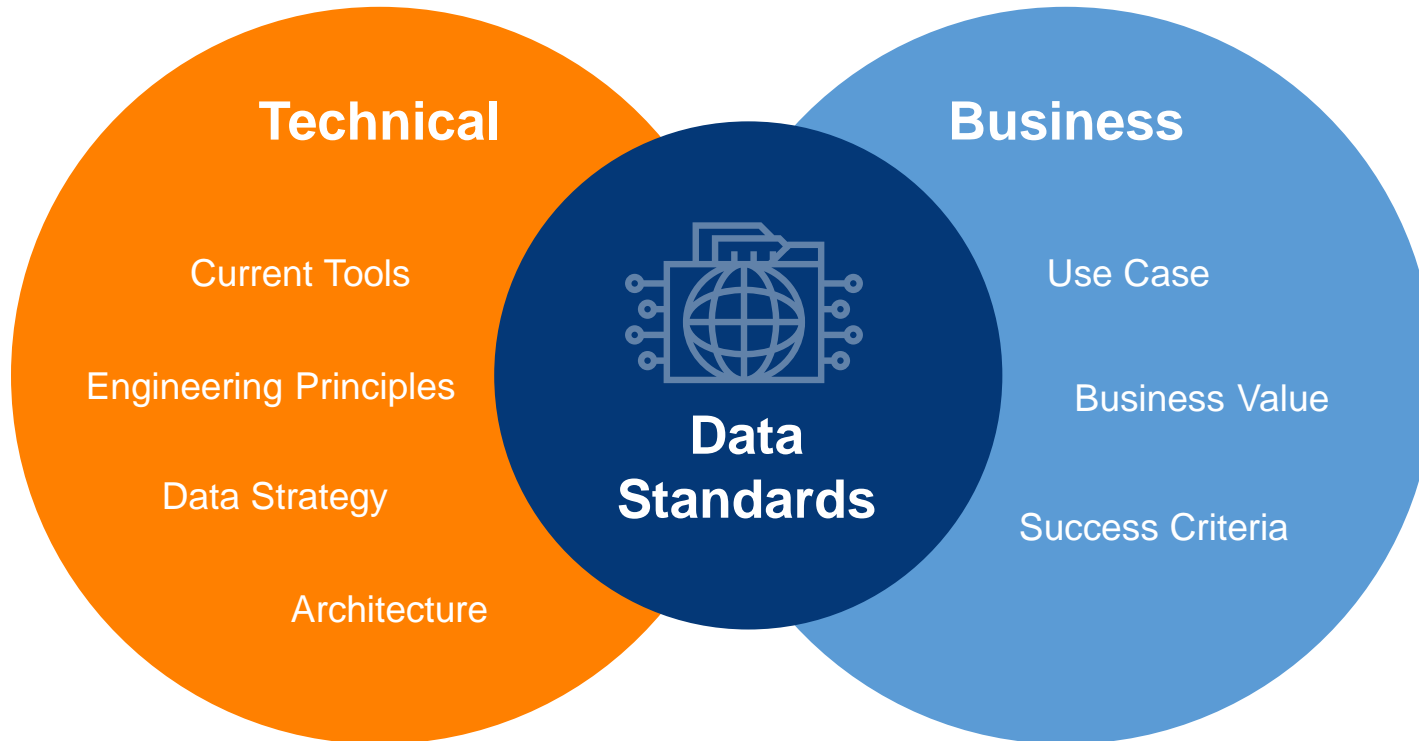
Technique	Sample JSON File	JSON Schema File
automated-reactors	automated-reactors.json	automated-reactors.embed.schema.json
balance	balance.json	balance.embed.schema.json
blood-gas-analysis	bga.json	bga.embed.schema.json
bulk-density	bulk-density.json	bulk-density.embed.schema.json
cell-counting	cell-counting.json	cell-counting.embed.schema.json
cell-culture-analyzer	cell-culture-analyzer.json	cell-culture-analyzer.embed.schema.json
code-reader	code-reader.json	code-reader.embed.schema.json
conductivity	conductivity.json	conductivity.embed.schema.json
disintegration	disintegration.json	disintegration.embed.schema.json
differential-scanning-calorimetry	differential-scanning-calorimetry.json	differential-scanning-calorimetry.embed.schema.json
dynamic-vapor-sorption	dvs.json	dvs.embed.schema.json
fluorescence	fluorescence-endpoint.json	fluorescence-endpoint.embed.schema.json
foam-height	foam-height.json	foam-height.embed.schema.json
foam-qualification	foam-qualification.json	foam-qualification.embed.schema.json
fourier-transform-infrared-spectroscopy	ftir.json	ftir.embed.schema.json
fast-protein-liquid-chromatography	fpic.tabular.json	fpic.tabular.embed.schema.json
gas-chromatography	gas-chromatography.tabular.json	gas-chromatography.tabular.embed.schema.json
gloss	gloss.json	gloss.embed.schema.json

<https://www.allotrope.org/asm>

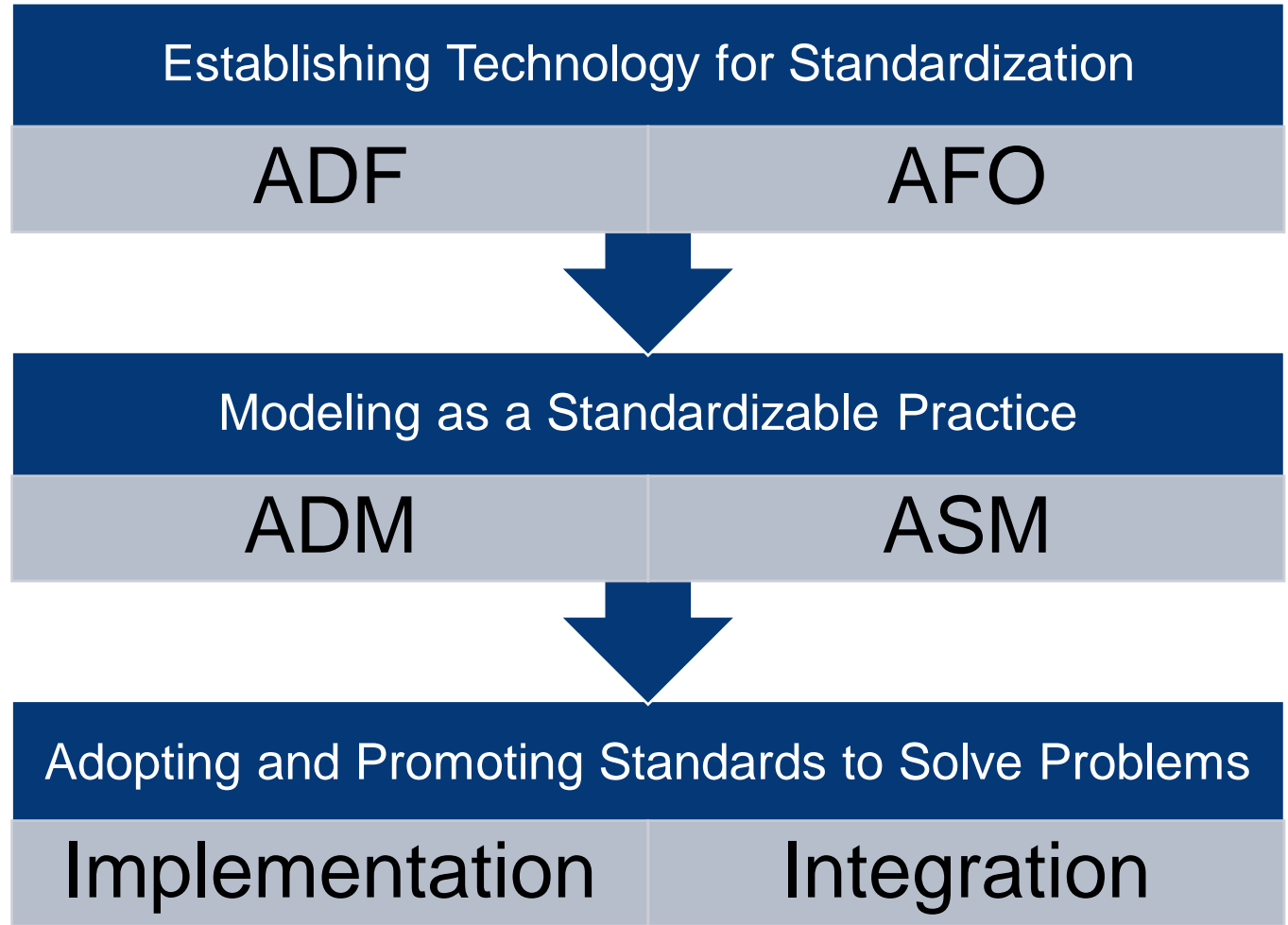
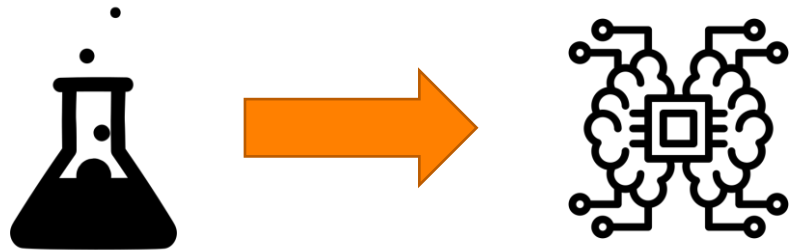
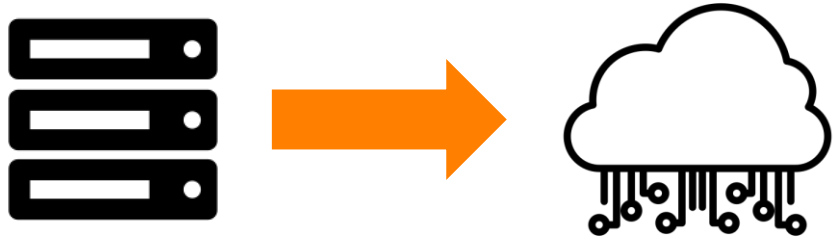


Establishing Data Standards as a Community

Allotrope works with other standards – and works as a community to solve data challenges



The Allotrope Journey



The Allotrope Community Today (as of March 29, 2023)

Allotrope Foundation



Allotrope Foundation Secretariat



Allotrope Partner Network Members

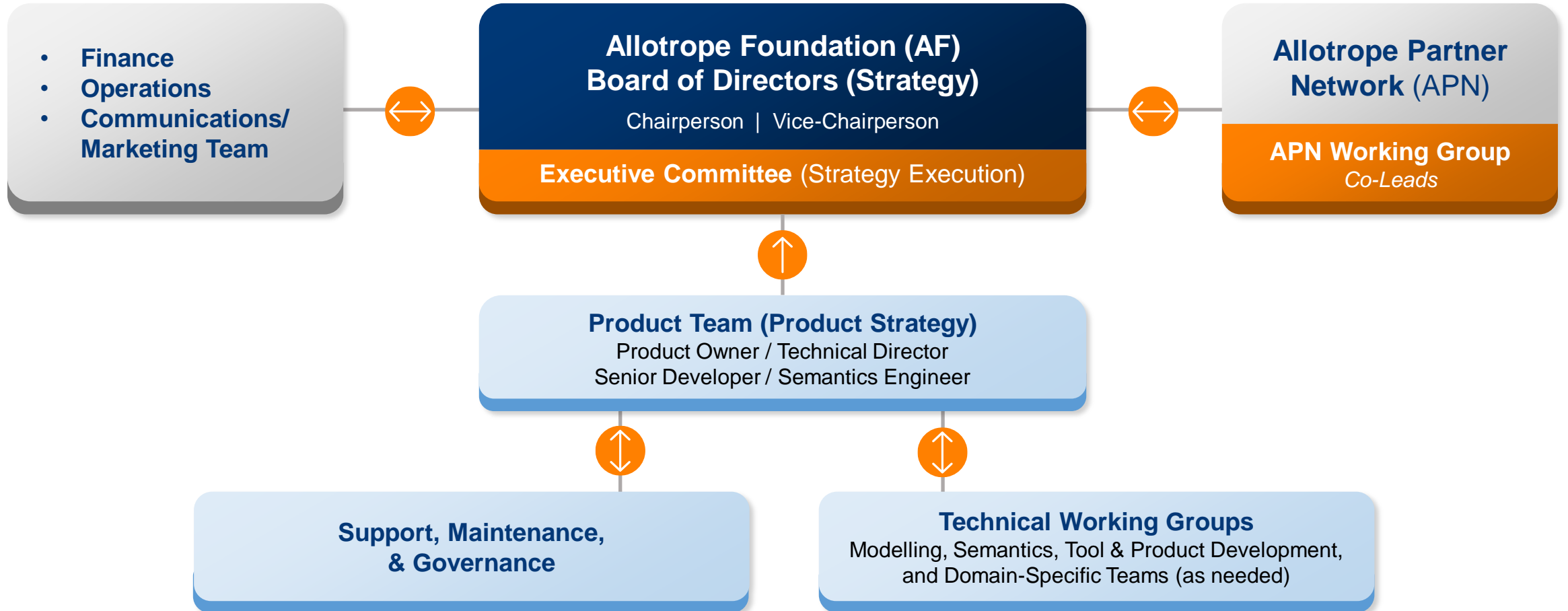


- Dotmatics
- Erasmus MC
- Fraunhofer IPA
- NIST
- Stanford University
- University of Illinois at Chicago
- University of Michigan
- University of Southampton



Allotrope Foundation Organizational Structure

A consortium managed by industry with dedicated product team



Agenda

- Day 1: Allotrope in Action (Public)
 - Presentations by members on Allotrope use in their own hands
- Day 2: A Community Focus on Adoption (Allotrope Members & APN)
 - Community meetings focusing on implementation and adoption of Allotrope, lessons learned, and exploring new opportunities
- Day 3: Moving Allotrope Forward (Allotrope Members & APN)
 - Working Group meetings, Technical office hours and discussions, Board meeting





Allotrope In Summary



Allotrope Data Models (ADM) and Allotrope Data Format (ADF) provide semantically-rich & interconnected data when you need it



A true community-driven standard driven by use cases, representing over 50 organizations



Allotrope Foundation Ontology (AFO) provides a common terminology foundation across techniques / domains



Allotrope Simple Models (ASM) make it easy to get started in any environment and solve many problems

