# Welcome to Allotrope Connect Spring 2023

Rethinking Scientific Data

Allotrope Foundation®

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

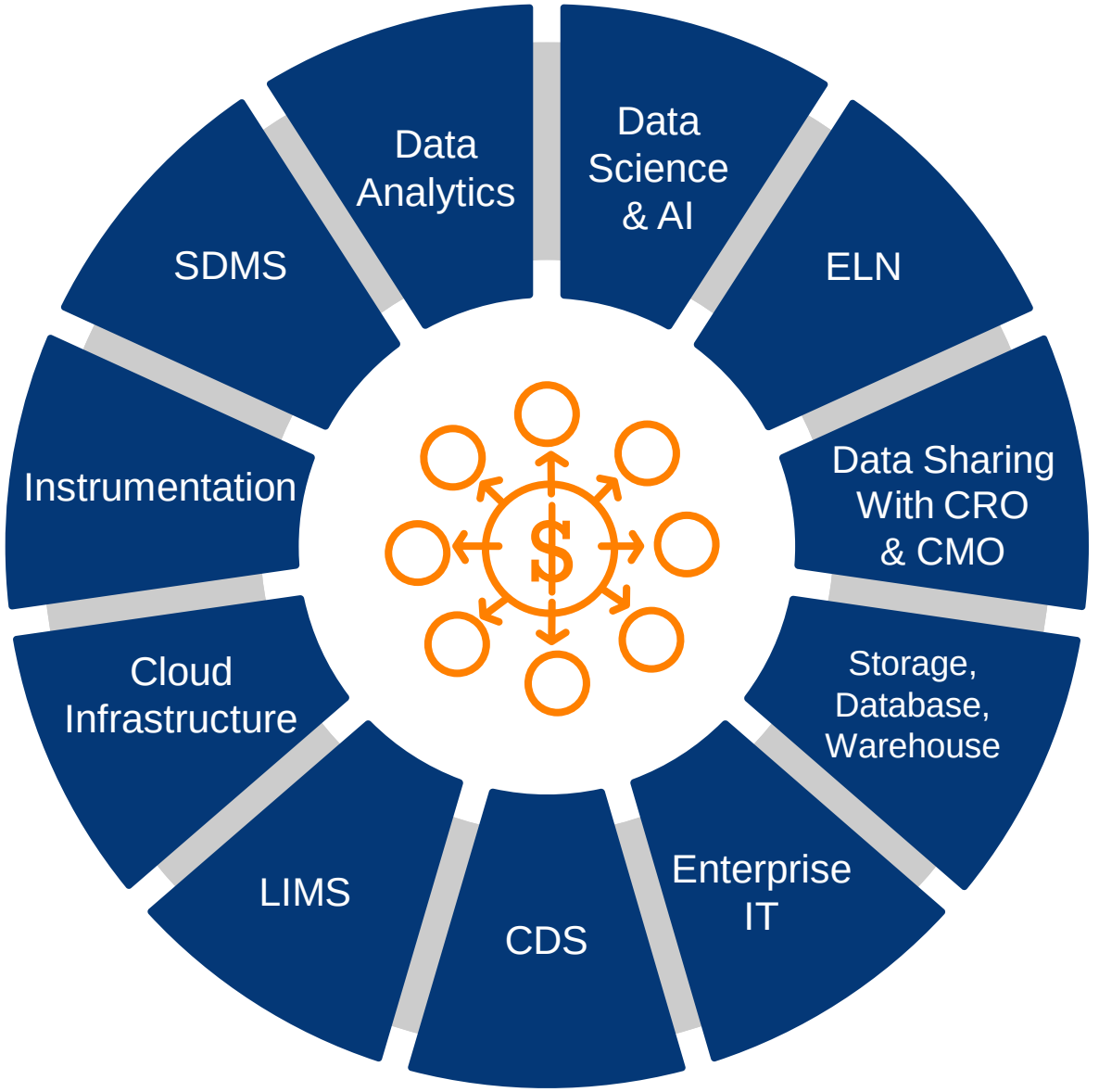
Data Centricity

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

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# 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

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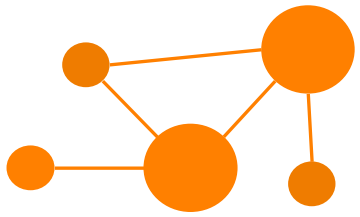
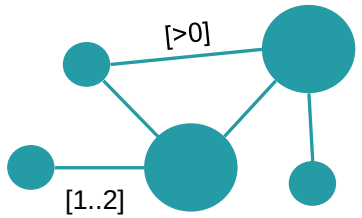
# Allotrope Framework Products



## AFO

### Allotrope Foundation Ontologies

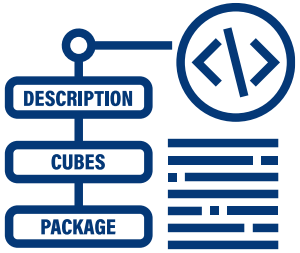
Defines terms & their relationships consistently across laboratory domains




## 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

## ASM

### Allotrope Simple Models

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

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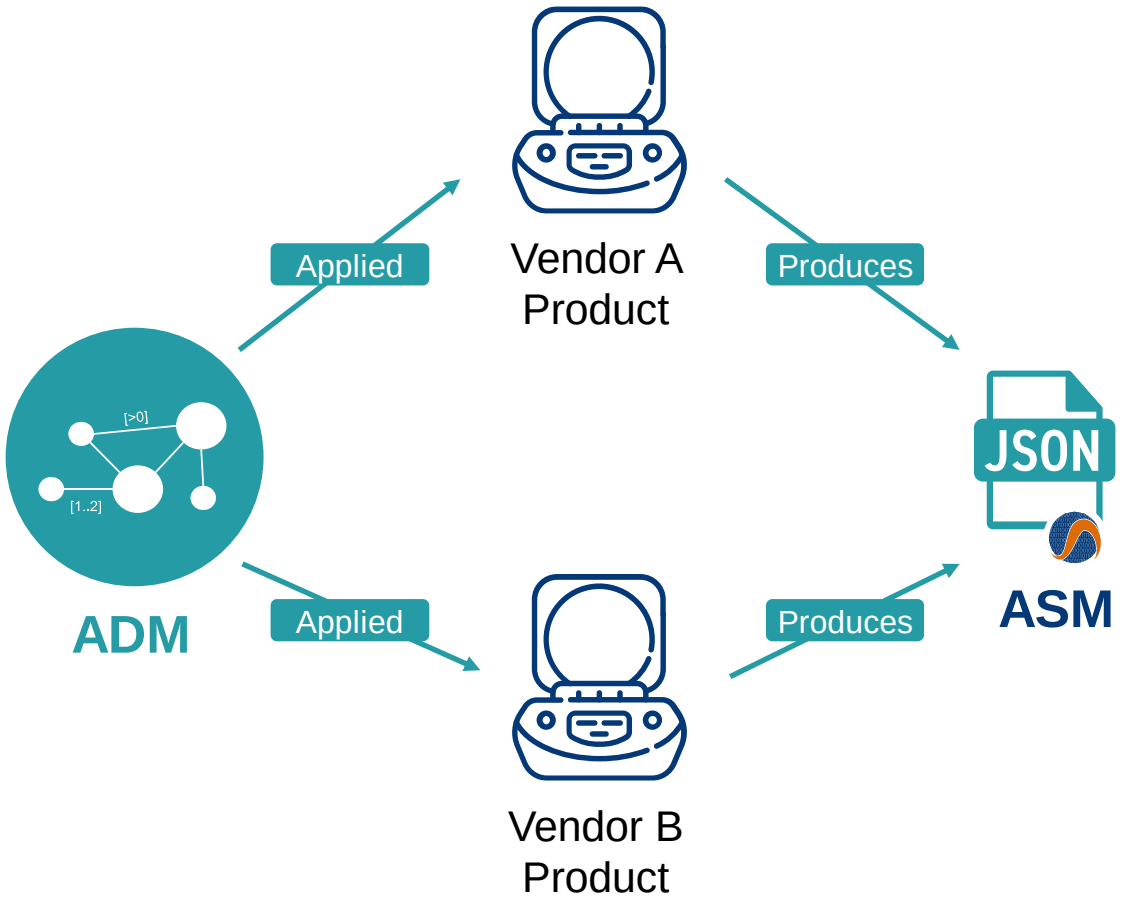
# Allotrope Data Models (ADM)

- 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

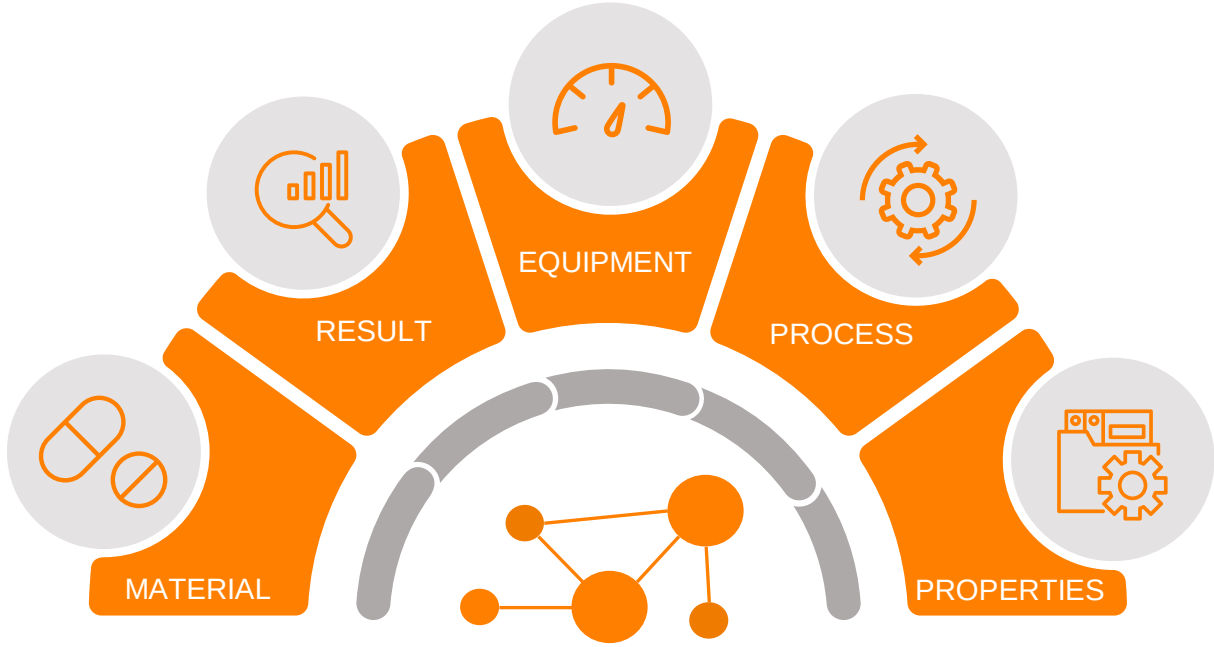
- Automated Reactors / PAT
- Dissolution
- **Liquid Chromatography***
- Oven/Coulumetric KF
- Specific Rotation
- Balance
- Blood Gas Analyzer
- Electrochemical Tester
- Liquid Particle Counter
- **pH Sensor***
- LC-MS
- Osmolality
- Surface Area Analysis
- Bulk Density
- **FPLC***
- Live-cell imaging
- 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
- Nepholometry
- **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




**AFO**

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"
  }
}
```

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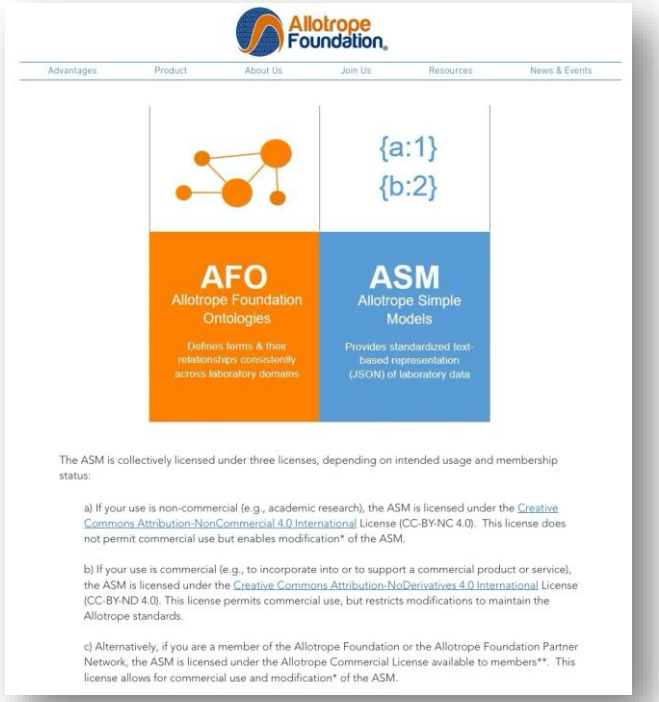
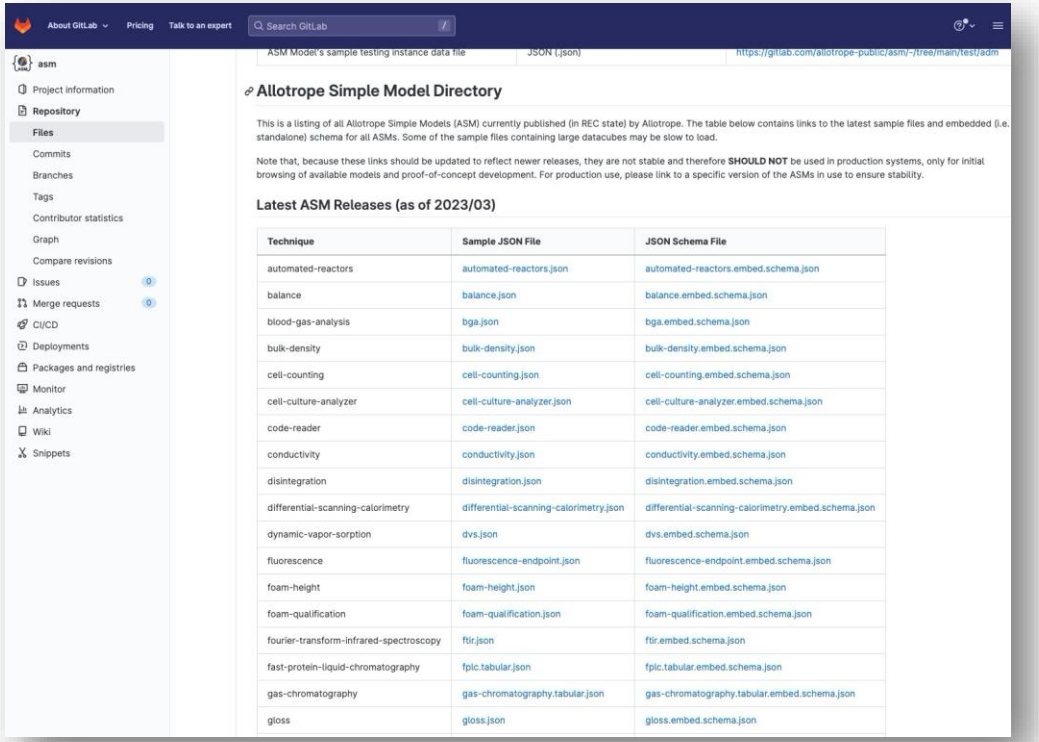
# Allotrope Simple Models are open to all!

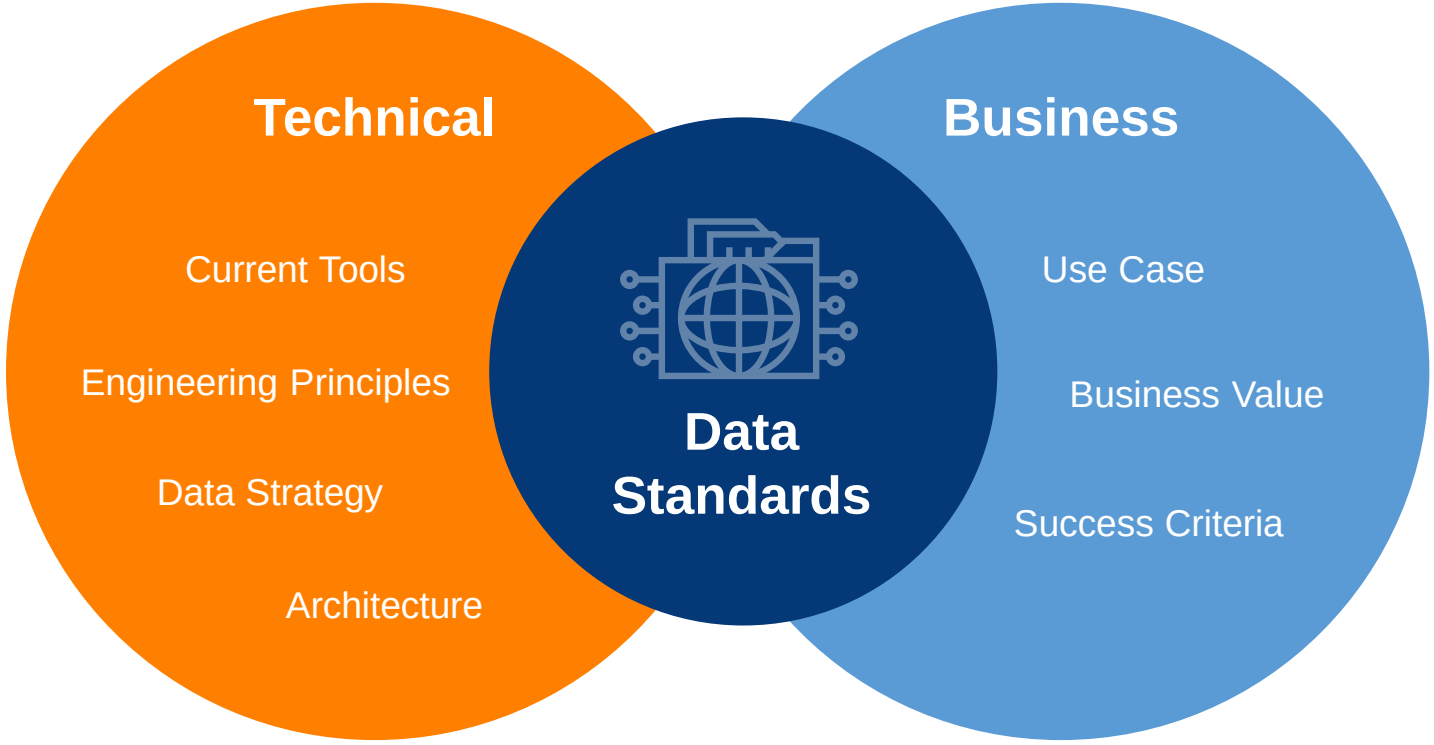


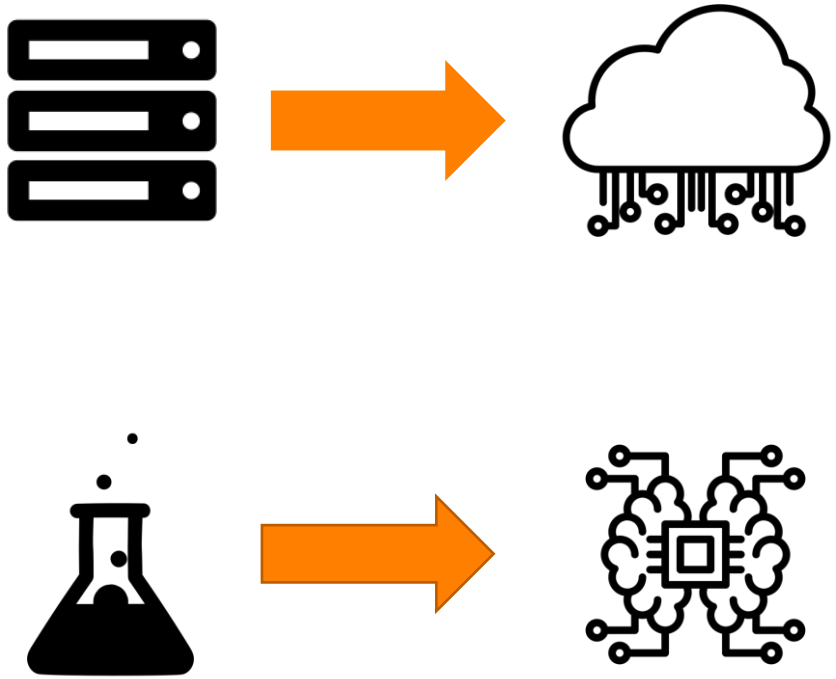

https://www.allotrope.org/asm

# Establishing Data Standards as a Community

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



# The Allotrope Journey



Establishing Technology for Standardization

ADF | AFO

Modeling as a Standardizable Practice

ADM | ASM

Adopting and Promoting Standards to Solve Problems

Implementation | Integration

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

## Allotrope Foundation

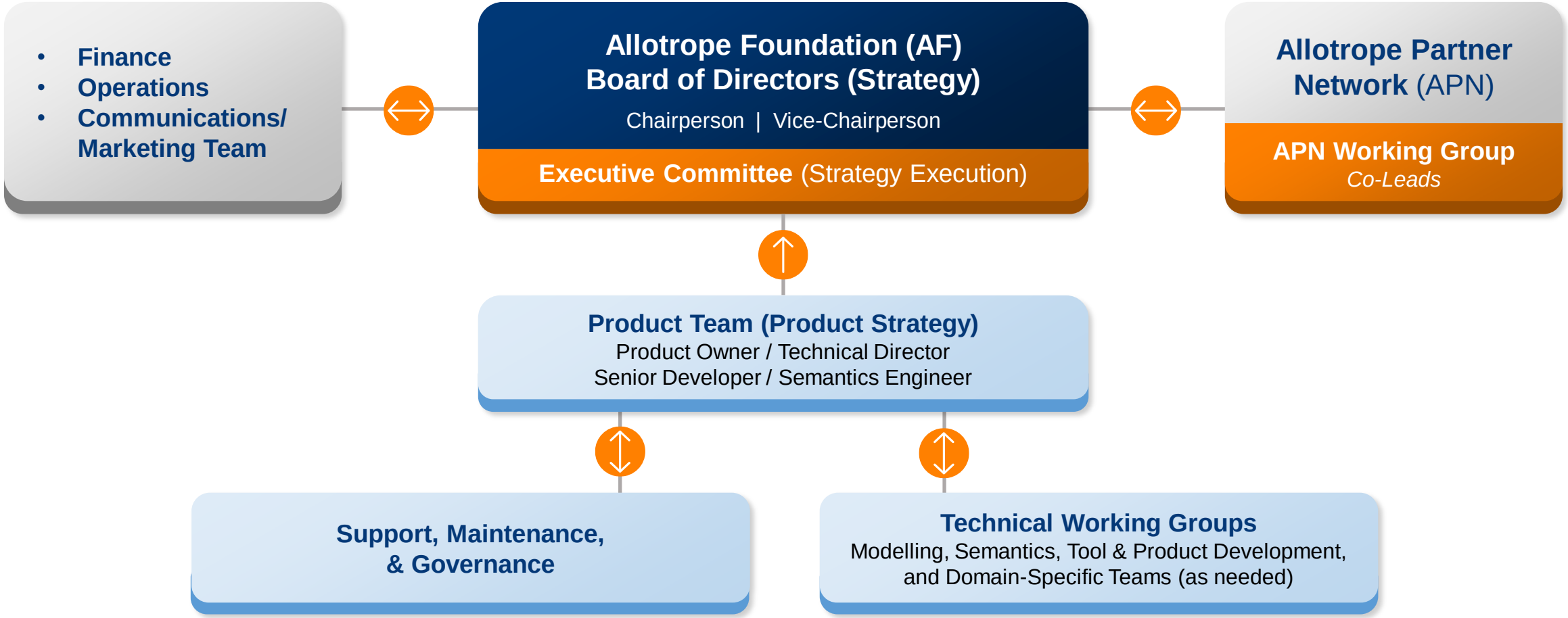
## Allotrope Foundation Secretariat

## 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