Working Groups, Release and Product Update

Update report by the Allotrope Product Team
2024 Fall Allotrope Connect Workshop

Update Agenda

- Quarterly Releases Updates
- DevOps Updates
- Working Groups Updates
  - Modeling WG
  - Chromatography WG
  - Mass Spectrometry WG
  - Plate Reader WG
  - Flow Cytometry WG
  - ELN WG

Quarterly Release Update

2024 Q2 + Q3 Releases

- New models including solution NMR, electrophoresis, and chromatography column
- Updated existing models including automated reactors, osmolality, and light obscuration

Q2

ASM Model	Type	Maturity	Path
Solution NMR	Tabular	REC	New
Electrophoresis	Tabular	REC	New
pH	Tabular	REC	Update
Balance	Tabular	REC	Update
Osmolality	Tabular	REC	Update
Automated reactors	Tabular	CR	Update
Plate readers kinetics (Absorbance, Fluorescence, Luminescence)	Tabular	REC	Update
Chromatography column	Tabular	CR	New
Core updates	Tabular	REC	Update

Q3

ASM Model	Type	Maturity	Path
Rheology	Tabular	REC	New
Light obscuration (as a Solution Analyzer detector)	Tabular	REC	Update
Automated reactors	Tabular	REC	Promoted from CR
Chromatography column	Tabular	REC	Promoted from CR
Electronic spectrometry (renamed from Spectrometry)	Tabular	REC	Update
GC-MS	Tabular	REC	New

LABLICATE peak efficiency
MERCK INVENTING FOR LIFE
BASF We create chemistry
Benchling

2024/Q3 Release

2024 Q3 release of the AFO and ASM is available on:

- GitLab,
- ASM Public Repo,
- PURL,
- JFrog,
- Client Connect
- Allotrope website (Wix)

- 2024/09 release of the AFO is also available on external Ontology Lookup Services:
  - BioPortal (AFO)
    - BioPortal, the repository of biomedical ontologies published by the National Center for Biomedical Ontology at Stanford University
  - Ontobee (AFO)
    - Ontobee, Ontologies data server published by the University of Michigan Medical School
    - Ontobee generates the AFO list of terms in an Excel spreadsheet as well as Tab Separated Values file
  - OLS4 (AFO)
    - OLS4, the Ontology Lookup Service repository for biomedical ontologies published by the European Bioinformatics Institute

- Automated
- Manual

ASM Modularization Continues
Using Common Hierarchy Schema

- ASM modularization work continues across the different working groups
- The Common Hierarchy Schemas is a collection of “Lego” like, reusable building blocks to create consistent hierarchical structures across the different models


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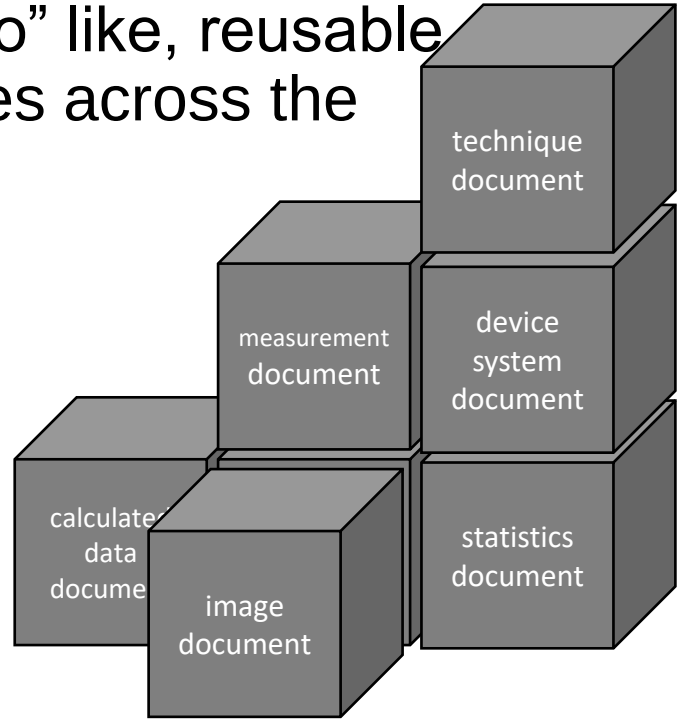
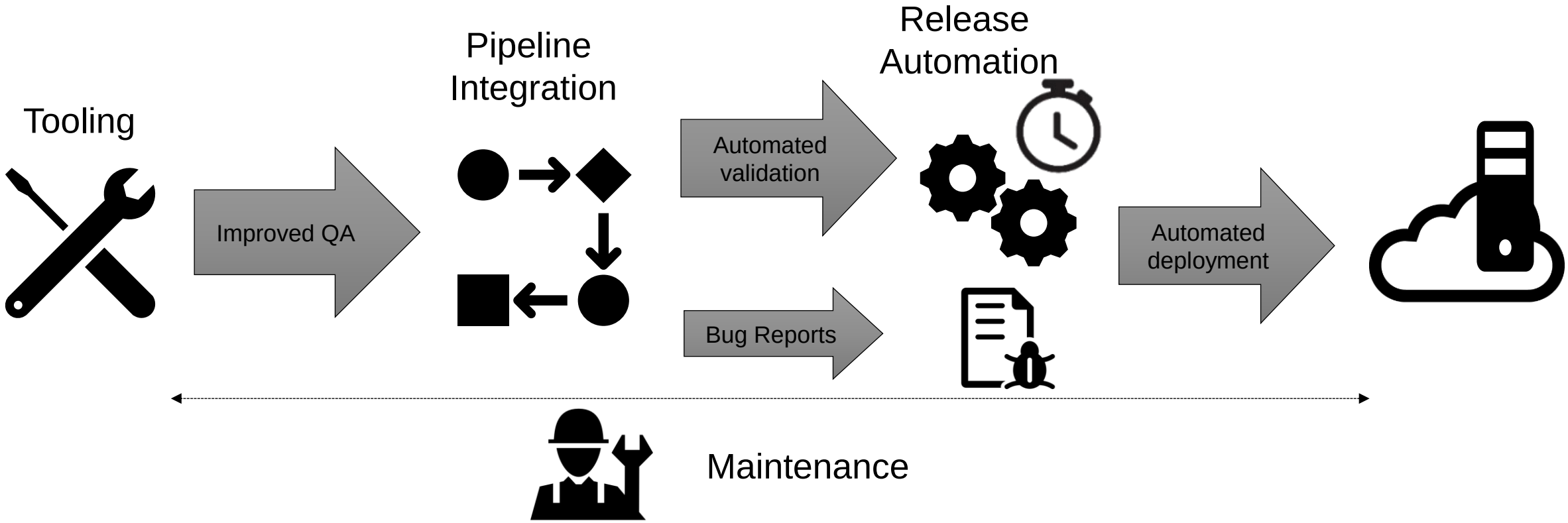
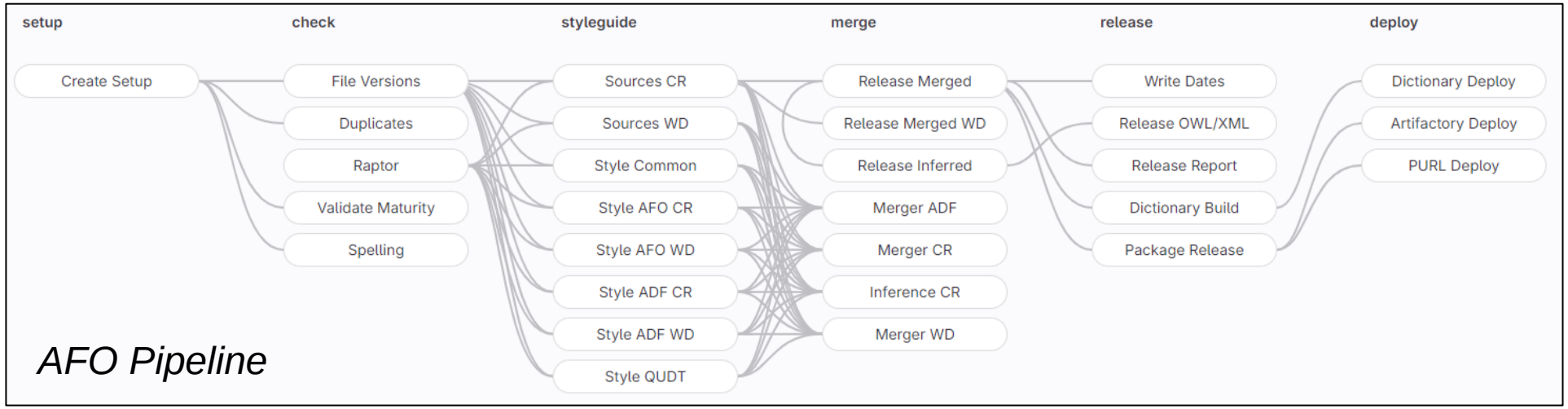


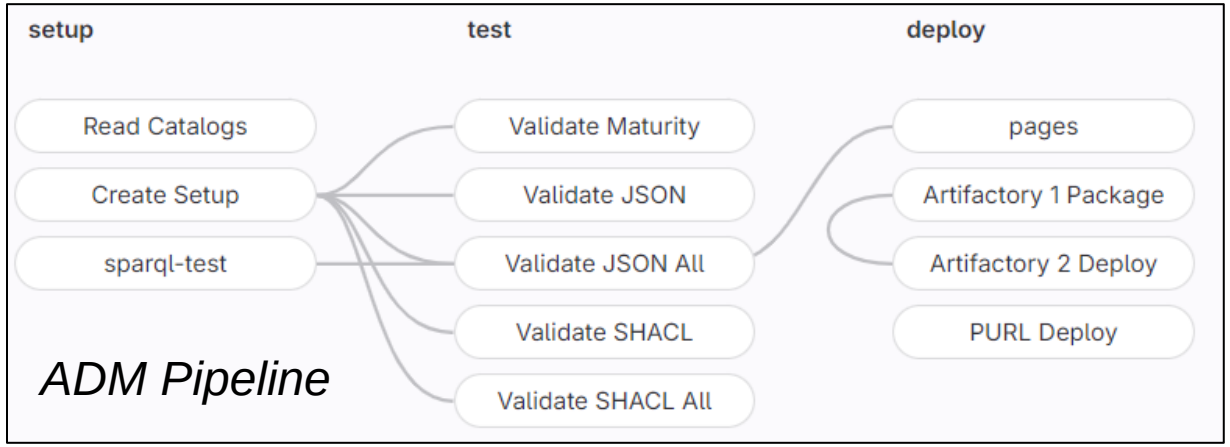
DevOps Update

The Big Picture: Streamlining the "Ontology and Model Development Lifecycle"
Scalable, Efficient, Automated, Up to Date and Collaborative



CI/CD Pipelines





- AFO pipeline:
  - https://gitlab.com/allotrope/afo/-/ci/editor?tab=1
- ADM pipeline:
  - https://gitlab.com/allotrope/adm/-/ci/editor?tab=1

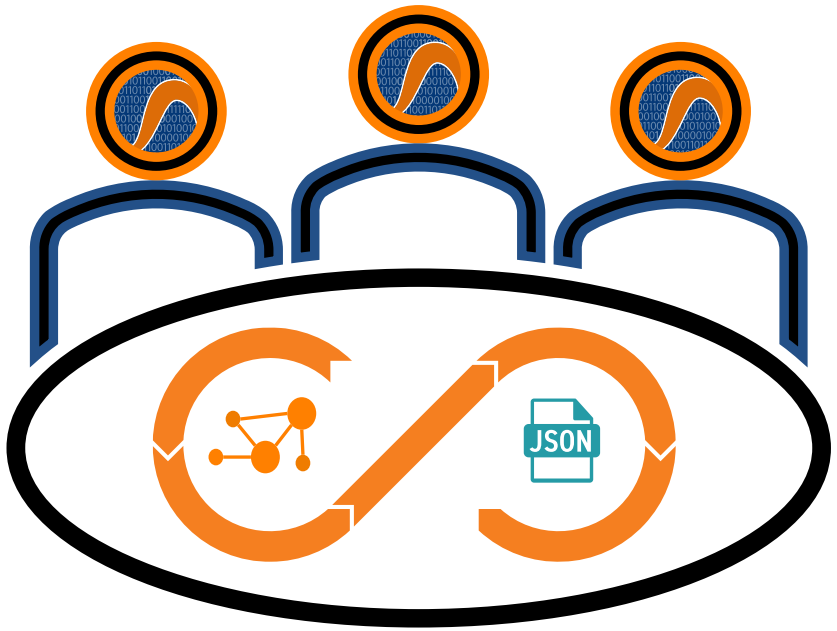
Maintenance Work

PURL (AFO server)

Maintenance

- Improving PURL (AFO server) stability
  - Update Fuseki (SPARQL server) to latest version
  - Resolve Fuseki (SPARQL server) database disk space consumption with every update
- Enable HTTPS on AF PURL server
- Align the AFO/ADM versioning with Git
  - Reduced repository size and enables use of standard Git tooling for diffs, history tracking
- QA enhancements
  - Add format checking to ASM
  - Check ASM manifests import existing AFO files

Working Groups Update



#	Name	Day / Time (EDT)	Frequency	Description
01	Modeling	Wed 11am	Weekly	Provides a single forum for the development and governance of new models/domains proposed by the Allotrope Community. The focus is on new tabular models with the minimum necessary to contextualize data and to interpret results from
02	Chromatography	Mon 11am	Bi-weekly	Technical discussions and modeling related to Chromatography.
03	Mass Spectrometry	Tue 10am	Bi-weekly	Technical discussions and modeling related to Mass Spectrometry.
04	Plate Reader	Thu 11am	Bi-weekly	Technical discussions and modeling related to Plate Readers.
05	Flow Cytometry	Fri 11am	Bi-weekly	Technical discussions and modeling related to Flow Cytometry.
06	ELN (Electronic Lab Notebook)	Fri 9am	Weekly	Technical discussion related to experiment authoring domain and data recording by Electronic Lab Notebook
07	Allotrope Partner Network	Tue 11am	Monthly on the fourth Tuesday	Discussions related to Allotrope strategy from an APN perspective.

Modeling WG

Weekly on Wednesday: 11am – 12pm ET

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Modeling WG Update

2024 Q2/Q3:

3 New models:

- Solution NMR (REC)
- Electrophoresis (REC)
- Rheology (REC)

6 Model updates:

- pH (REC)
- Balance (REC)
- Osmolality (REC)
- Automated Reactors (REC)
- Light Obscuration (REC)
- Electronic Spectrometry (REC)

2024 Q4:

- Binding Affinity (Benchling)
  - Initial detector to be SPR (Surface plasmon resonance)
  - Potential new pattern for externalized datacubes under discussion

2025+:

- Calibration model
  - Device
  - Measurement
- Multi-Angle Light Scattering (Merck)
- Liquid handlers (Benchling)
- Imaging/Optical Microscopy update (Benchling)
- X-ray diffraction update (BASF)

Chromatography WG

Bi-Weekly on Monday: 11am – 12pm ET

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Chrom WG Update

2024 Q2/Q3

1 new model:

- Chromatography Column (REC)

Review of 2 models:

- Electrophoresis (Benchling/Merck)
  - Reviewed at the Chrom WG and governed at the Modeling WG
- GC-MS (Lablicate)
  - Reviewed at the Chrom WG and governed at the MS WG

2024 Q4

- Reviewing chromatography modularization
  - Expanding a common core for chromatography (chromatography model)
  - Discuss improving how inheritance works, (per Matthias' view) could be a major shift

2025+:

- Multi-Angle Light Scattering (Merck)
- Size Exclusion Chromatography (Merck)
- Supercritical Fluid Chromatography (GSK)
- Possible adding gradients
  - Temperature gradient - controlled increase of the column temperature during the separation process
  - Solvent gradient - gradual change in the composition of the mobile phase (solvent) over time during the separation process.

Mass Spectrometry WG

Bi-Weekly on Tuesday: 10am – 11am ET

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Mass Spec WG Update

2024 Q2/Q3

1 new model:

- GC-MS (REC)
  - Bringing GC model and MS detector modules together, with additional scaffolding
  - Clarified handling of datacubes for large, sparse MS data in ASM and ADF

2024 Q4

- The MS WG is adding Ionization types terms to the ontology
  - There is no current, well structured ontological classification for ionization type.
  - Current sources include CHMO, PSI-MS, and OBI
    - These tend to be either incomplete or internally inconsistent

2025+:

- MALDI-TOF extensions to the existing MS model (Lablicate)
- MS-MS model (Lablicate)

Plate Reader WG

Bi-Weekly on Thursday: 11am – 12pm ET

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Plate Reader WG Update

2024 Q2/Q3

Model extension:

- Kinetics reads (Absorbance, Fluorescence, and Luminescence)
  - The reading or measurement of kinetic data in a plate reader.
  - In plate readers, a kinetics read involves taking measurements at multiple time points to observe changes in a sample over time.

2024 Q4

- Spectral scans
  - Extending absorbance and fluorescence models to support scans over a spectrum of wavelengths
- Benchling presented a draft schema for optical-imaging to enable florescence detection where the results includes an image
  - Submitted a draft proposal that includes support for capturing of fluorescence and transmitted light imaging/microscopy (separate measurement schemas)

2025+:

- Area scans (use in immunology/biology)
- Optical Spectrometry terms
  - Introduce the 'spectrogram' and 'spectrogram data cube vs Introduce a generic 'spectrum' and 'spectrum data cube’

Flow Cytometry WG

Bi-Weekly on Friday: 11am – 12pm ET

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Flow Cytometry WG Update

2024 Q2/Q3

- Review of the existing space to define scope
  - FCS is the de-facto standard for individual measurements
  - Recording gating and the analysis is less well defined; this is where we can bring value

2024 Q4

- Working towards resolution/alignment of ASM model
  - Acquiring and understanding example data
  - Incorporation of data regions for capturing gating analysis

2025+:

- First release of flow cytometry model
- Spectral cytometry (Merck)

ELN WG

Weekly on Friday: 9am – 10am ET

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ELN WG Update

2024 Q4

- Team formed
- Established scope of initial model usecase
  - Archiving complete ELN entries to a datalake
- Merck/Zontal provided initial model to capture this data
  - Highly generic model, minimal semantic information
  - Intent to align this with Allotrope patterns for a CR release in Q4

2025 Q1-Q2:

- Design spec to extend archiving model with semantic annotations and key metadata recorded in a more concrete, user-friendly way
- Start PoC of the extended model to prove out the patterns and confirm what additional metadata should be included

2025 Q3+:

- Push extended model to CR release based on PoC outcomes

Thank You!

Allotrope Product Team