AnIML From 30,000 Ft

What is AnIML? What can I do with it?

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BSSN Software

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Overview

- Motivation
- Introduction to the AnIML data standard
- AnIML Use Cases
  - Archiving
  - Generic Software
  - Integration
- Summary

Introduction to the AnIML Data Standard

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Outline of AnIML

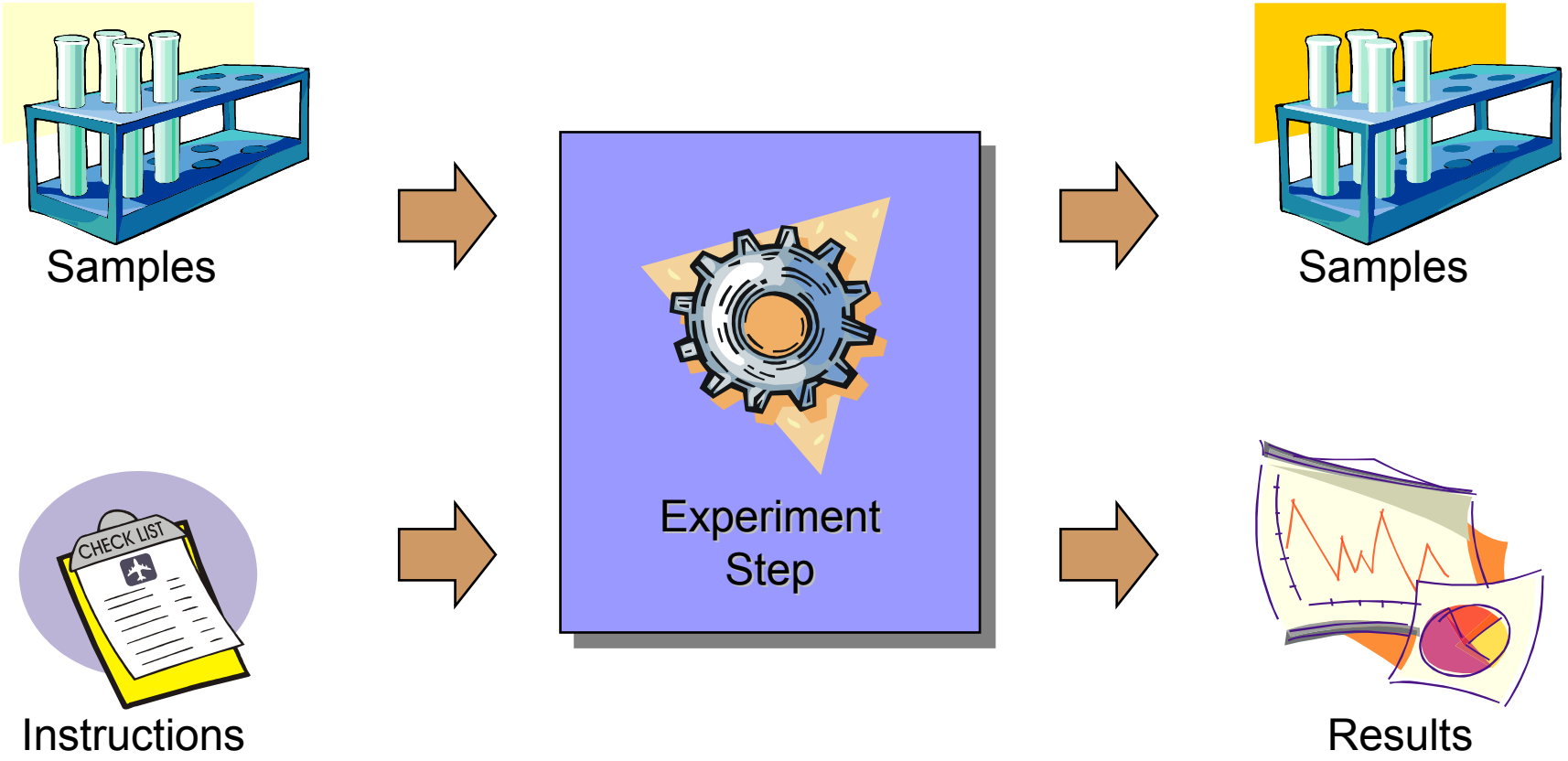
- Analytical Information Markup Language
- Upcoming ASTM XML standard for analytical data, developed by a consortium of industry, academia, vendors, and government bodies

- **Core** provides generic data container to represent “arbitrary” analytical data
- **Technique Definitions** explain how to use the Core for specific techniques

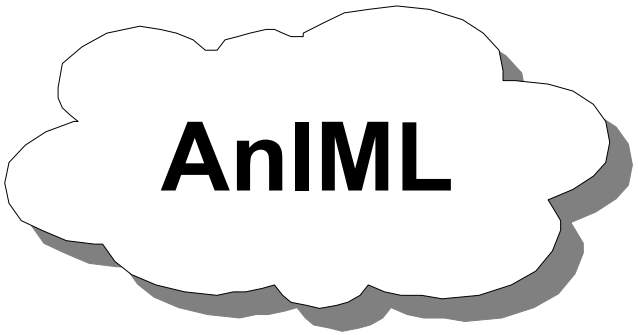
AnIML Design Goals

- Ability to capture data from multiple analytical techniques, possibly combined
- Capturing of sample and process data
- Room for extension by vendors and end users
- Audit trails, digital signatures, and validation for regulatory compliance

AnIML Experiment Model

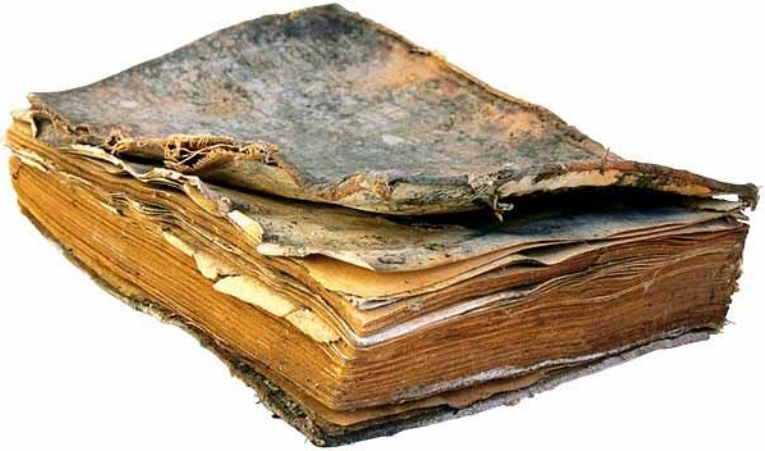


Possible Roles of AnIML



- Interactive viewing
- Instrument integration
  - Commodity techniques
  - One-offs and custom hardware

- Data management
- Data analysis
- Long-term archiving
- Result delivery
- Publishing, “open access”
- Regulatory submissions



Optimizing Long-Term Data Archival

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Long-Term Data Archival

- Many challenges to manage:
  - Repository and physical storage
  - Data format
  - Conversion tools
    - Needed as long as a particular source format is used
  - Software for data access
    - Needs to be deployed – and upgraded “forever”
  - Validation
    - Needed initially and with every upgrade
  - ...

Data Formats

- Every allowed data format constitutes a liability
- Software to read the format needs to be preserved as long as the format is current
- Long tail impacts total cost of ownership
- Why not PDF?
  - Stores text and image output, not the underlying data
  - Can not be post-processed

AnIML as an Archival Format

- Open specification
- Captures all required data across techniques:
  - Sample, method and workflow description
  - Instrument and operator
  - Results
  - Identifiers, tracking information (batch, lot, time, ...) to relate information back to original context
- Human readable, even without software tools
- Verbose

Software for Data Access

- “Less is more”
- One tool for any instrument and technique
  - Proprietary software not required
  - Less upgrades & associated re-validation
- Lightweight tool with restricted set of features
  - Low validation effort
- Combination of AnIML and unified archiving tools can reduce total cost of ownership

Leveraging Generic Software Applications

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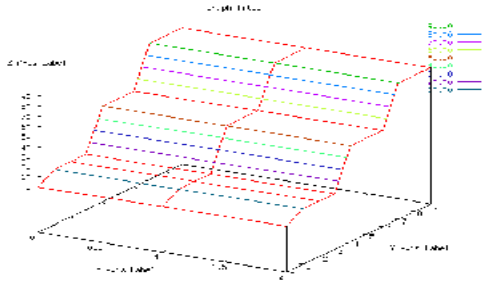
AnIML and Generic Software

- Many things can be done without understanding the underlying technique:
  - Displaying, reporting
  - Searching and querying
  - Validation and compliance
  - Digital signatures and audit trails
  - Long-term archival



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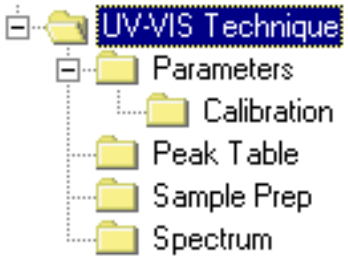
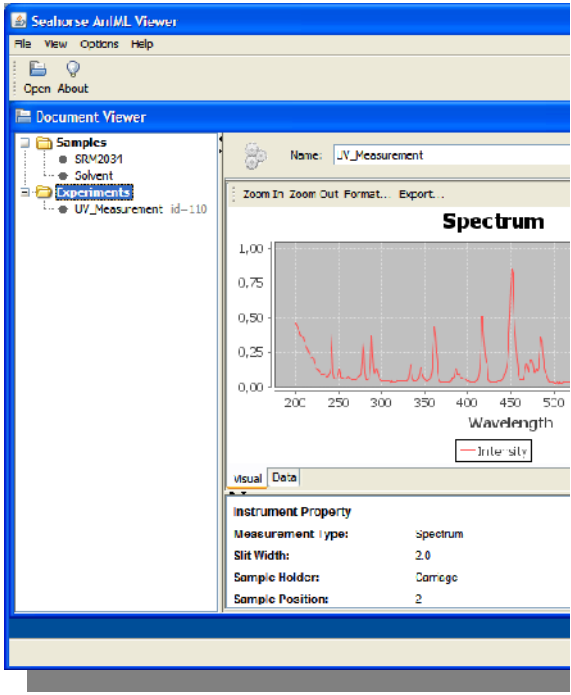
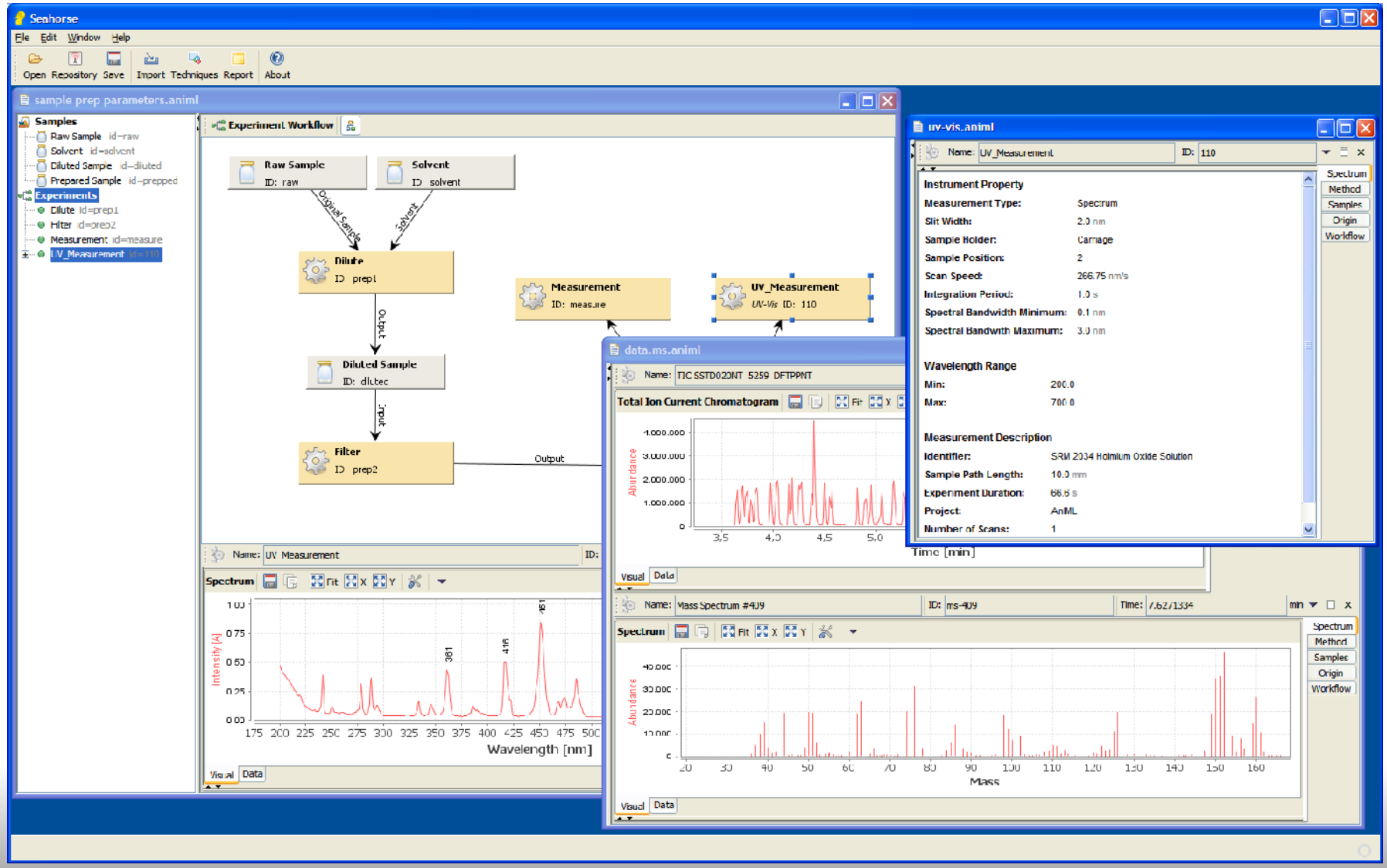


Benefits of using generic software components

- Proprietary instrument software is not required to view the data
- Only a compact set of software tools need to be deployed to end user PCs
- Viewing archived data requires only a single tool
- Software can be reused as new techniques are adopted



Seahorse Scientific Workbench



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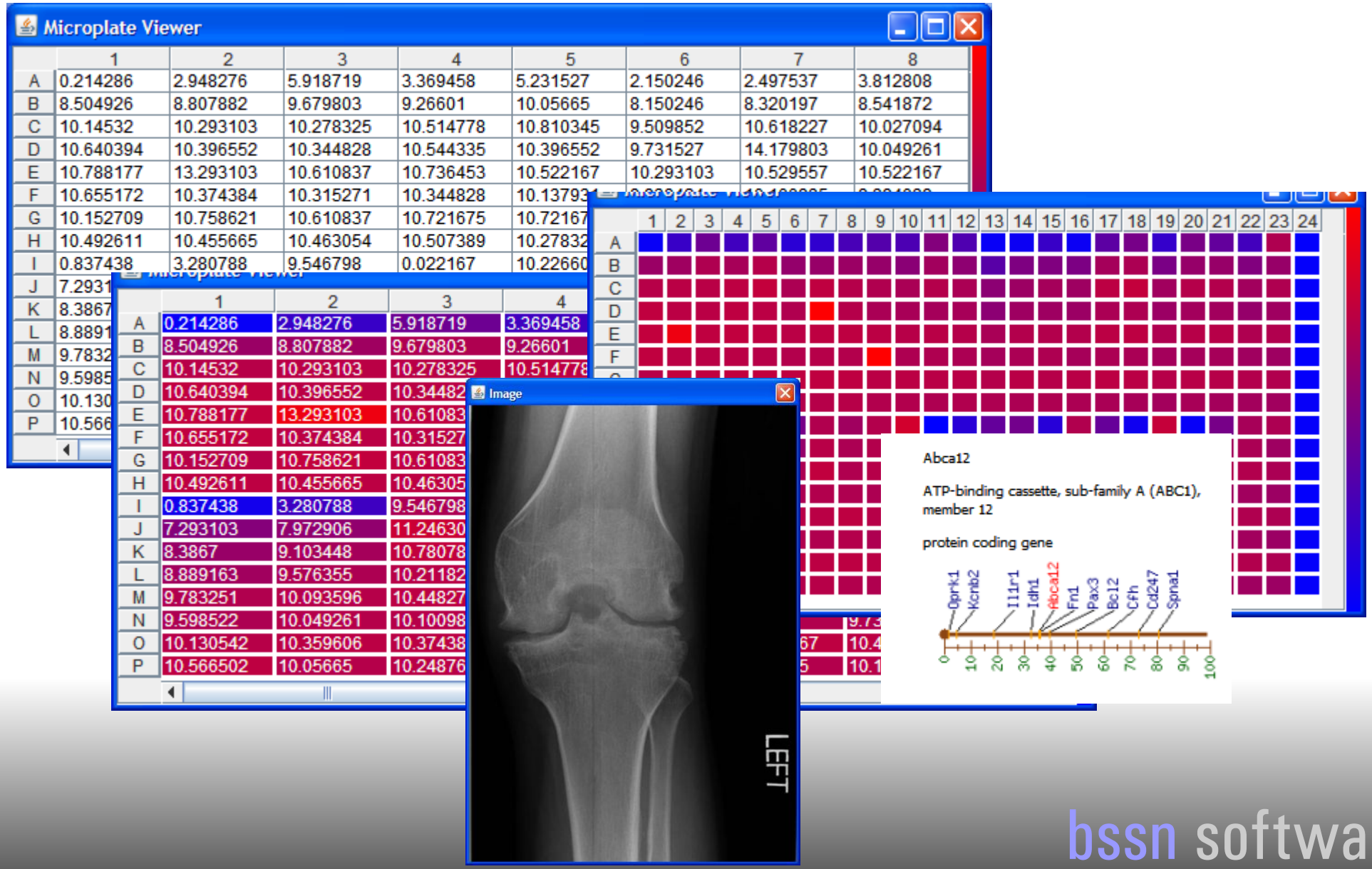
Seahorse Scientific Workbench



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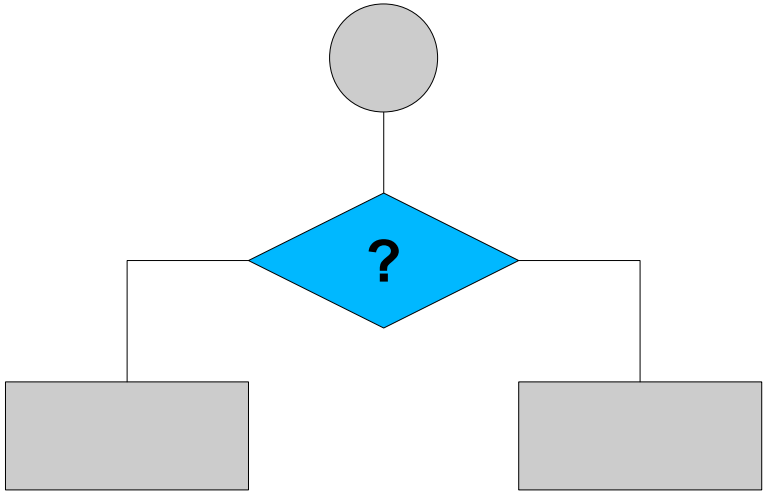
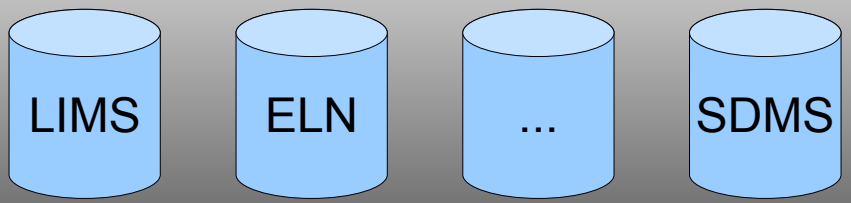


The Vision of Total Integration

Today's Instrument Integration

- Lab informatics landscape consists of many data producers and data consumers

Integration ?



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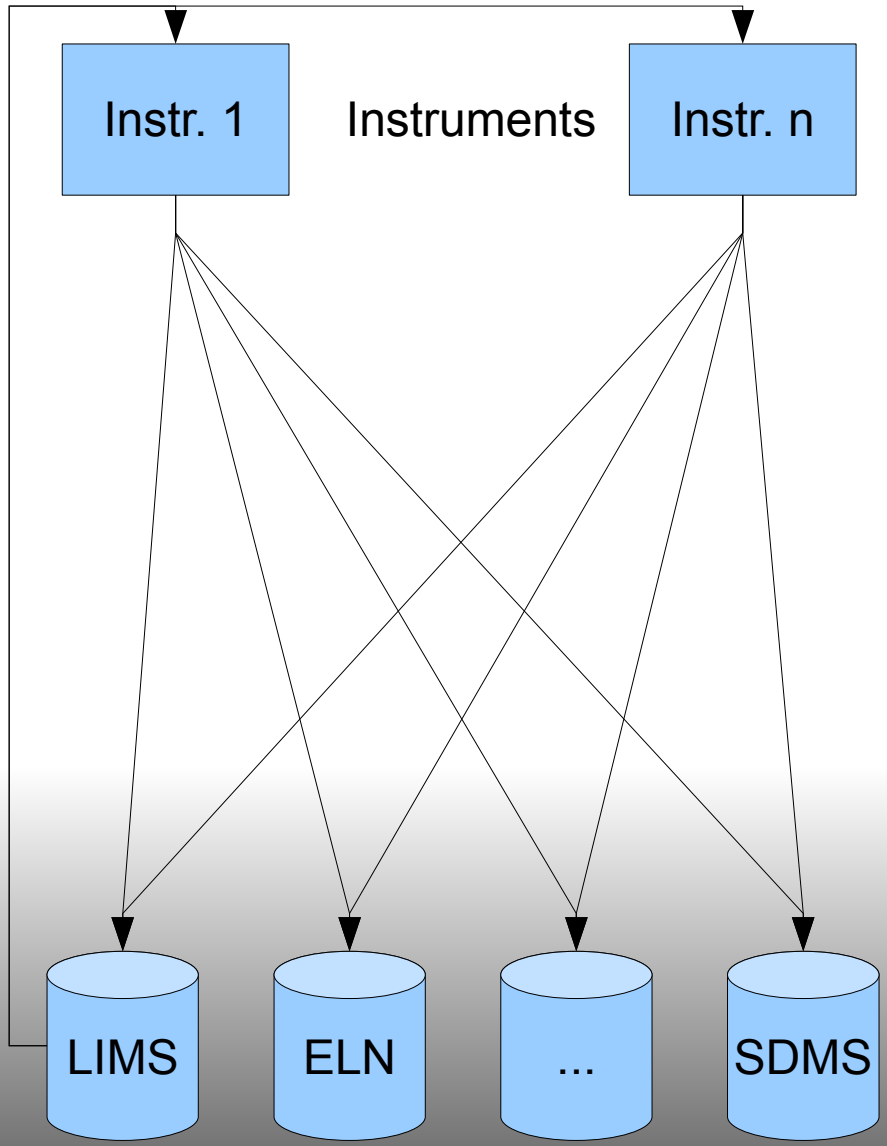
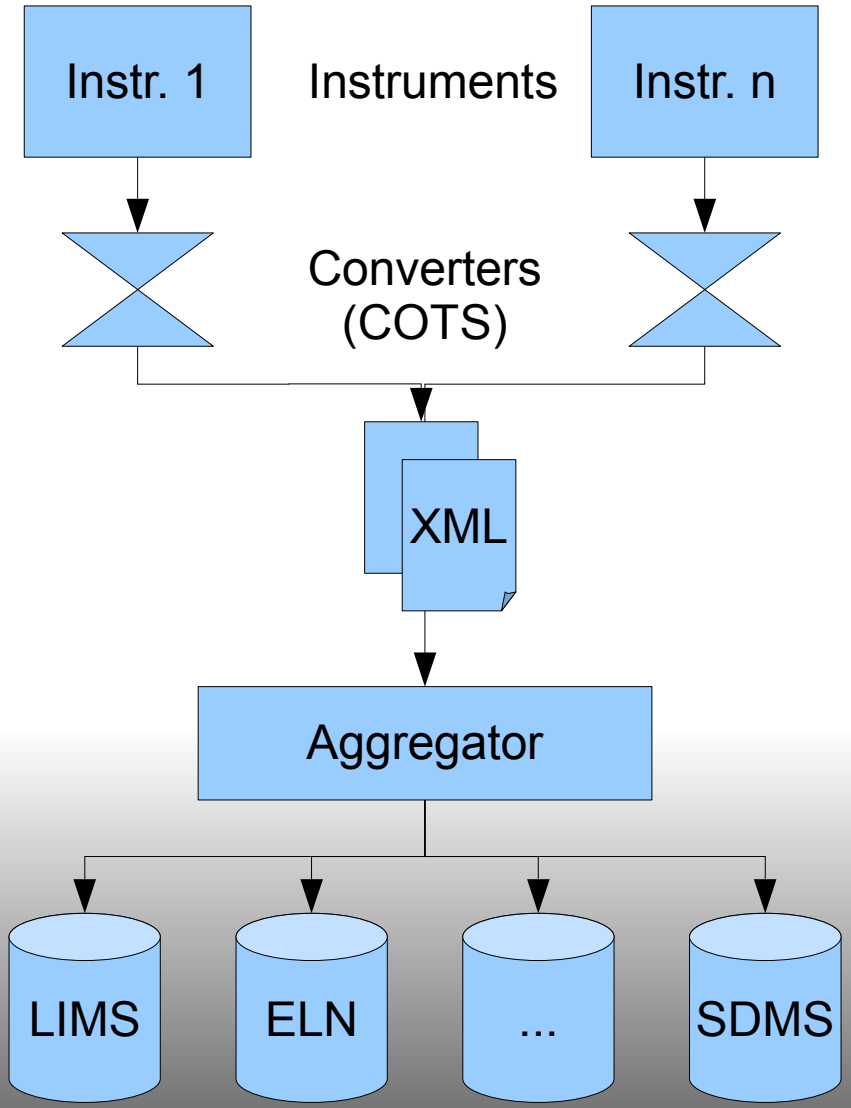
Today's Instrument Integration



- Lab informatics landscape consists of many data producers and data consumers
- Linking instruments and data systems often requires a 1-to-1 integration approach

Standards-Based Integration



- Instrument data is converted into AnIML
- Standard data is aggregated
- Target-specific fields are propagated to data systems
- Low n+1 cost

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Summary

- Adopting an open, standards-based approach to data management
  - Enables use of data in new ways
  - Delivers long-term business value
- A combination of AnIML and generic software tools can help us get closer to this goal

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What is AnIML? What can I do with it?

Live AnIML Showcase

Booth #5155

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