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Flexible Standardization with

AnIML

Technique Definitions

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For Complete Confidence

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Overview

- Basics
- Techniques
- Phase 1 Technique Definitions
- Extensions
- Sources of Information

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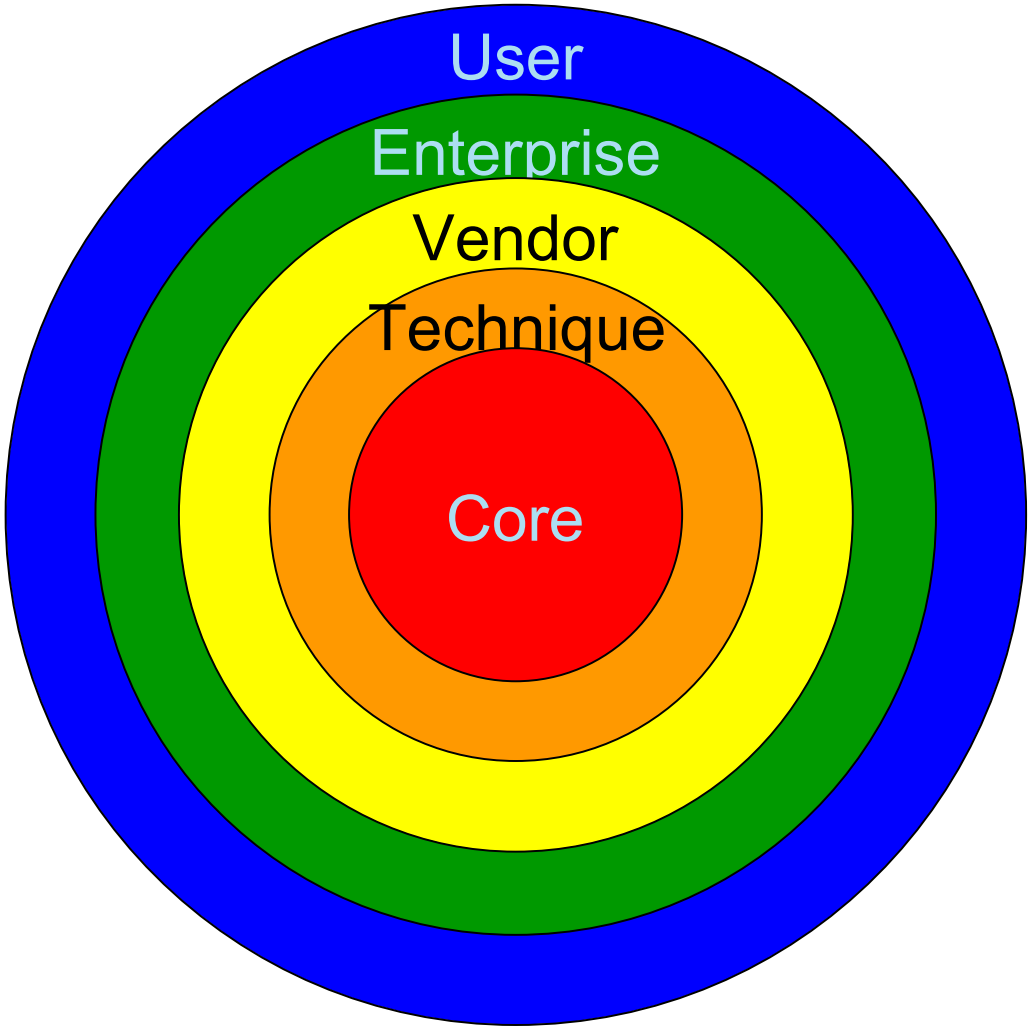
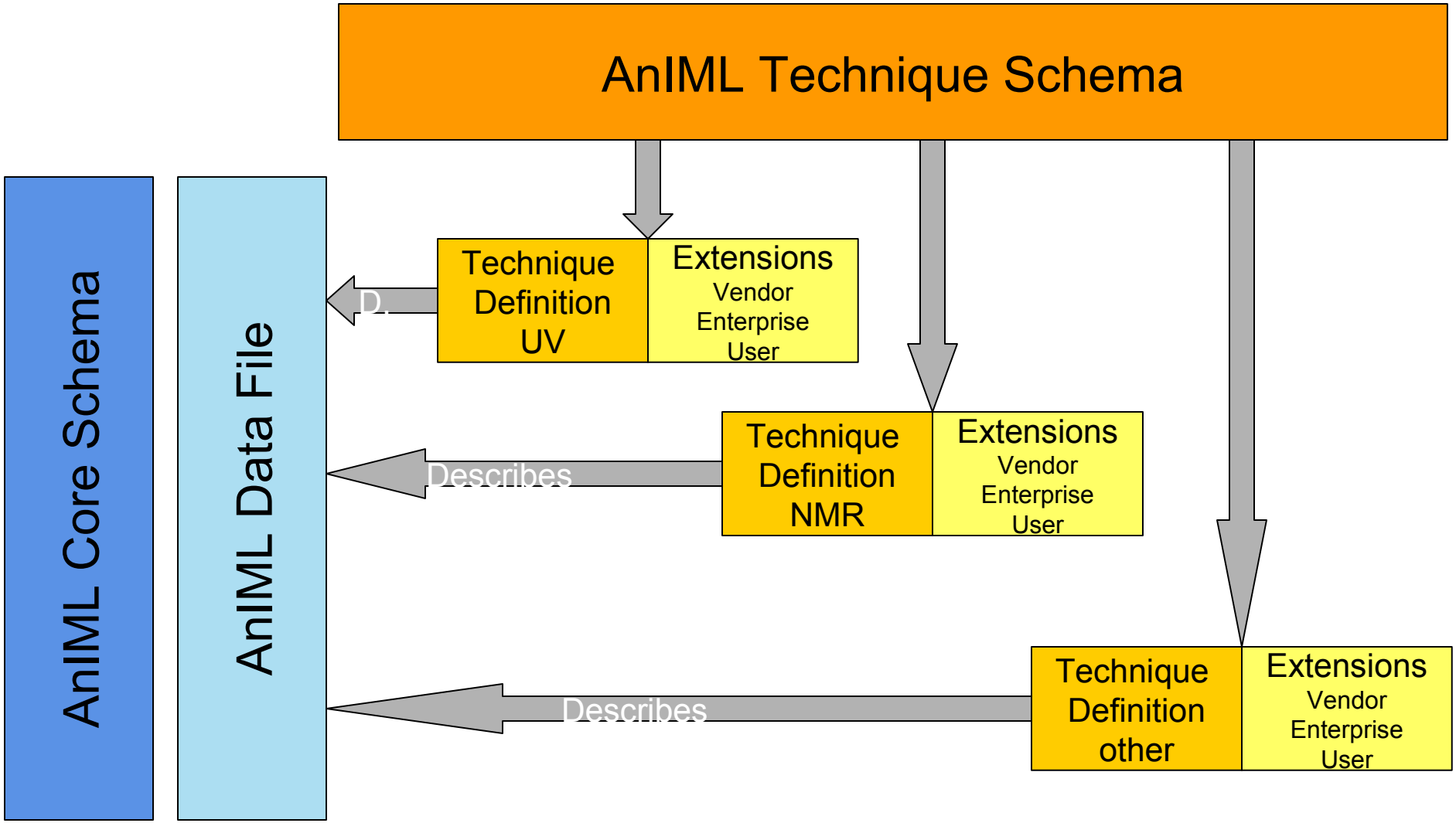
AnIML Conceptual Model





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Techniques

- Technique Definition Documents are XML instance documents adhering to the AnIML Technique Schema
- Technique Definitions explain *how to use* the Core for specific techniques
- Technique Definition prescribes
  - Ontology and data dictionary for a technique
  - Required and optional parameters
  - Parameter types, allowed values/ranges

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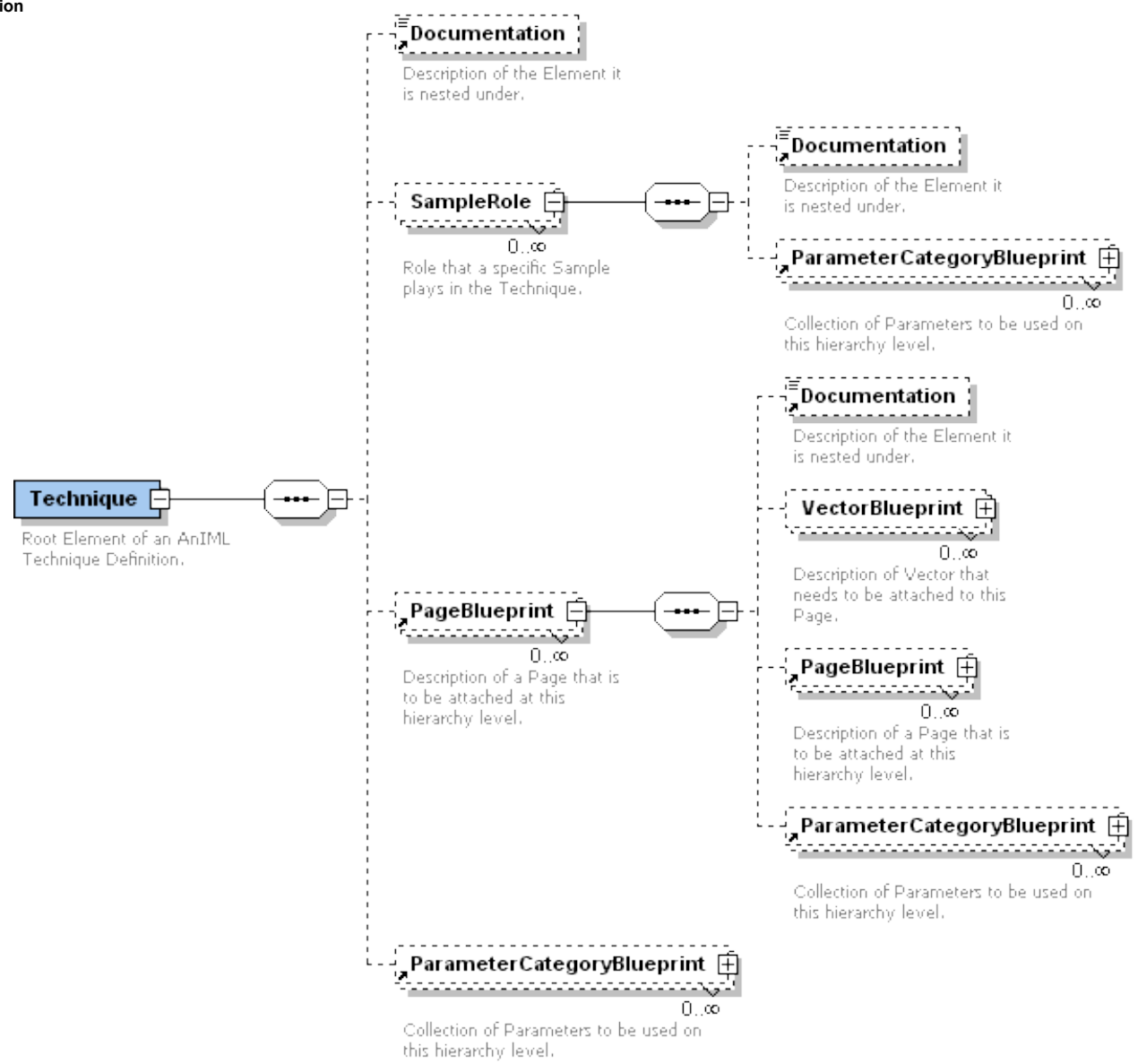
Technique Definitions



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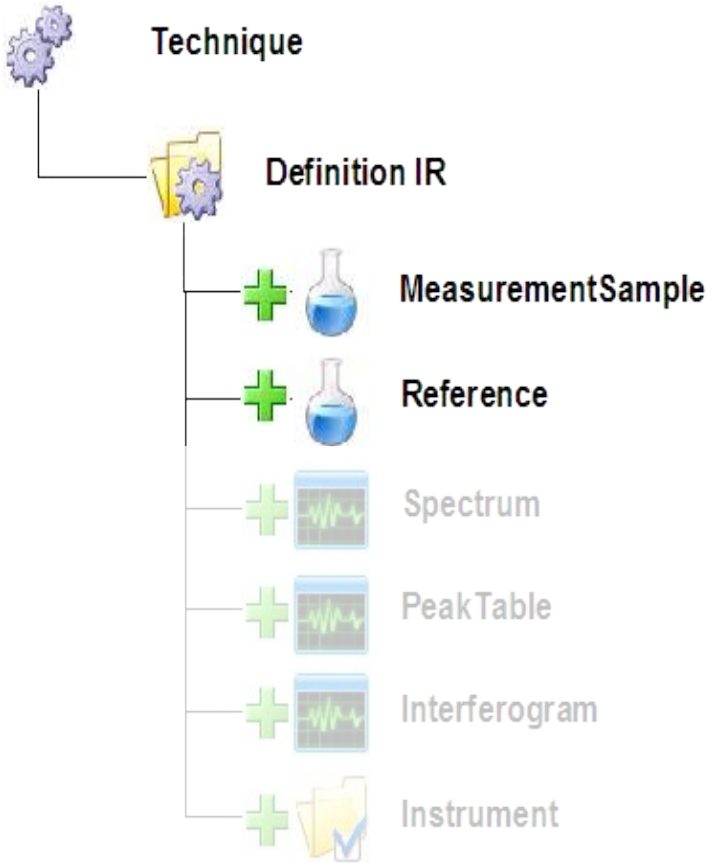
Samples

- Sample information is technique specific
- Sample Roles (e.g. calibration, run, blank...)
- Reuse by reference, inheritance
- Sub-sampling and sample flow (produced/consumed samples)



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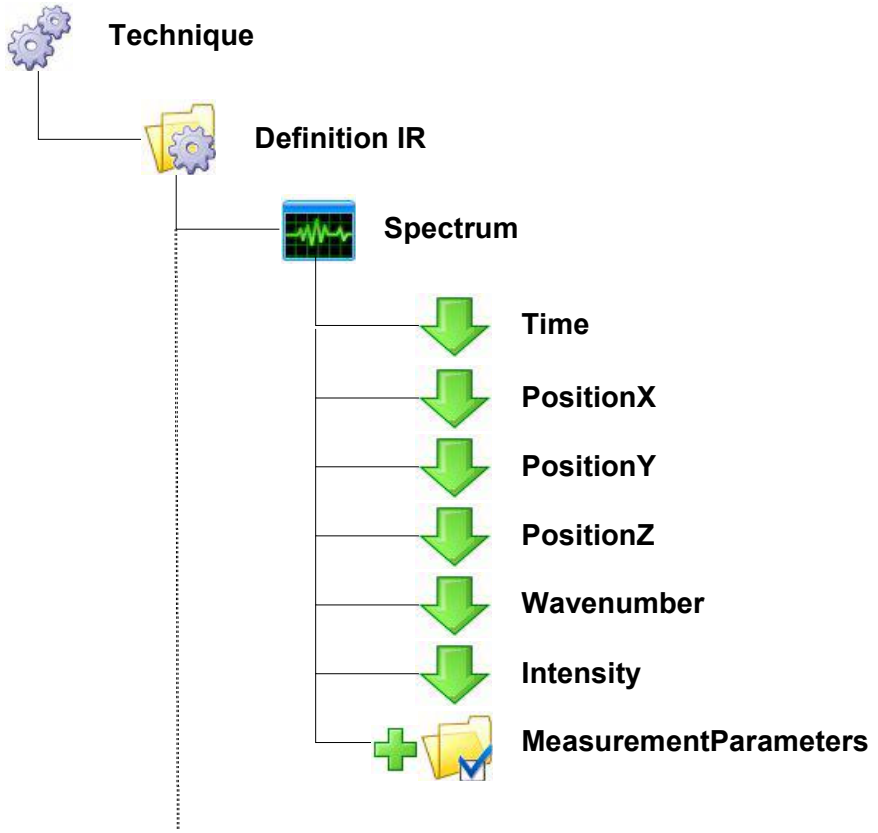
Page Blueprint

- Required and optional pages
- Required and optional vectors
- Vector value types
- Parameters



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Phase 1 AnIML Techniques

- UV/Vis
- NMR
- IR
- MS
- Chromatography
- IMS

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AnIML sources

- JCAMP-DX Elements
- ANDI Elements
- IUPAC Gold Book Definitions
- ASTM Terminology

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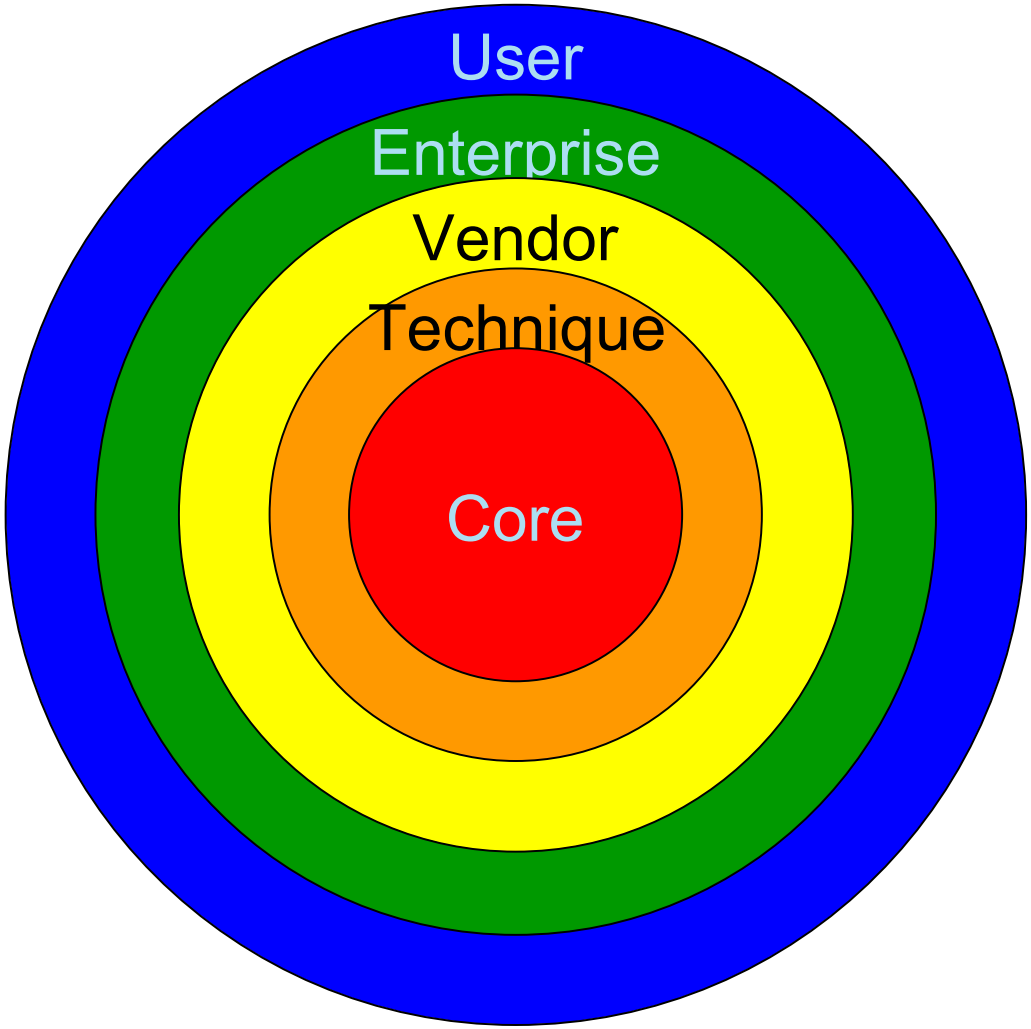
AnIML Conceptual Model



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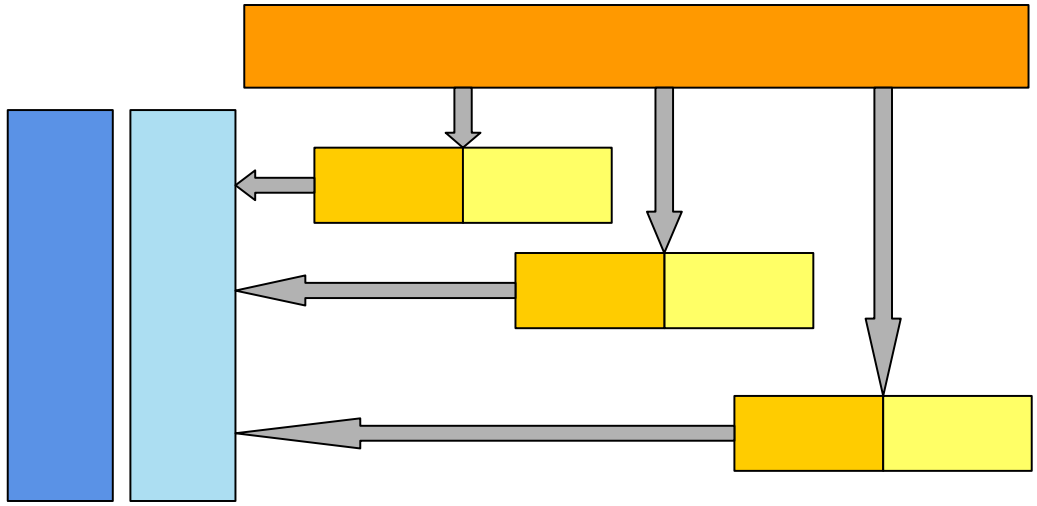
Extensions

- Technique Definitions can be amended using Extensions
- Used to define vendor- or user-specific additions to a Technique
- Stored in XML files (adhering to Technique Schema)
- Extensions “overlay” Technique Definitions
- Allows an arbitrary number of “shells”
- Does not break technique-specific applications



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Validation of AnIML documents

- Syntactic Validation
  - Checks Document Against Schemas
    - Format
    - Element Completeness
    - Data Types
- Semantic Validation
    - Correct Unit Types
    - Inclusion or Exclusion of Values in Sets
    - “Appropriateness”
    - NIST AnIML *Semantic Validator* Program
- Bounds/Limits Checking
    - Data ≤ or ≥ a Limiting Value
    - Data Between or Outside of Ranges of Values

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Sources of Information

- The AnIML Web Site
  - animl.sourceforge.net
  - www.animl.org

- The SourceForge Analytical Information Markup Language Project: Summary Page
  - sourceforge.net/projects/animl

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Help welcome!

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Q&A