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MXLIMS

for multi-sweep, multi-crystal experiments

Rasmus Fogh, Global Phasing

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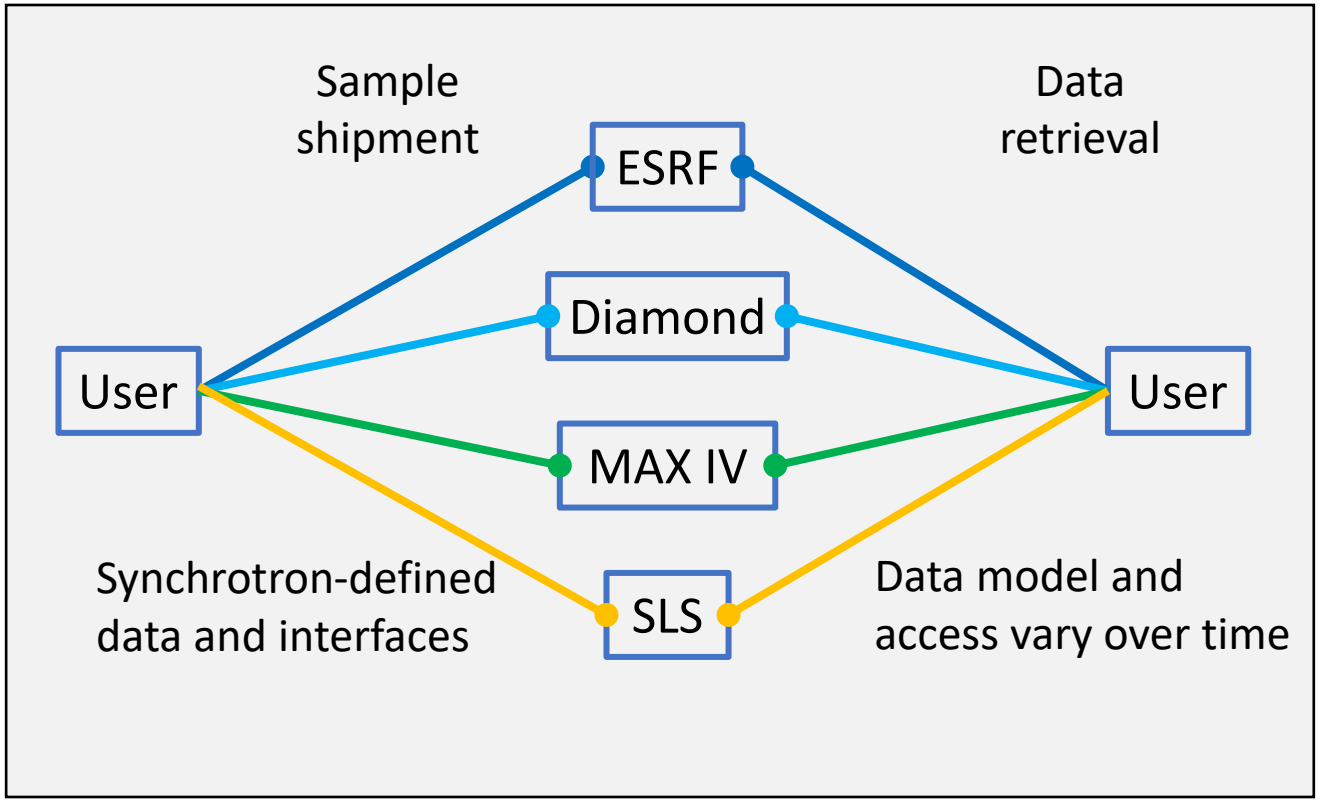
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- **MXLIMS Overview**
- Multi-sweep, multi-crystal facilities

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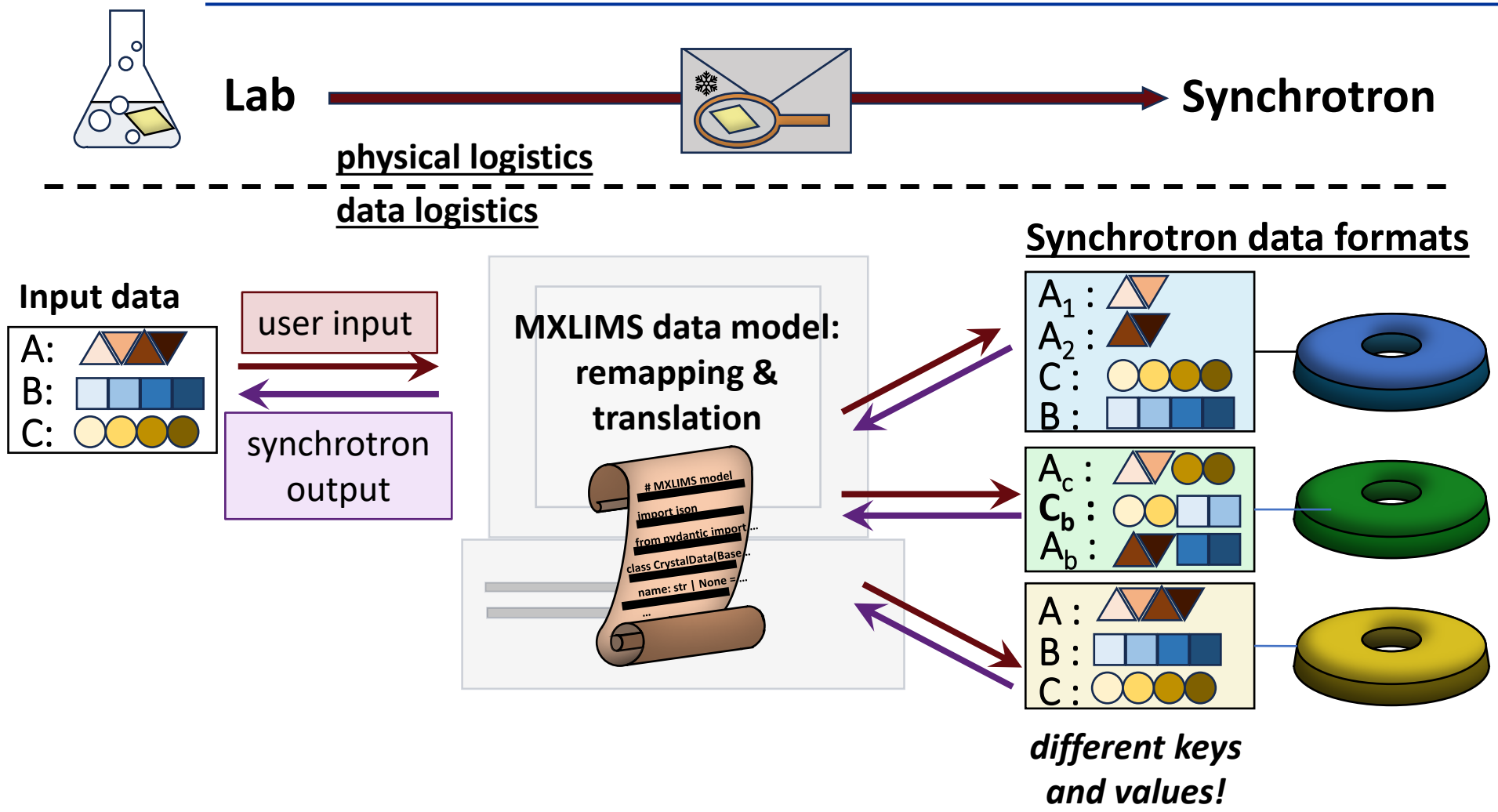
Shipping and data retrieval - now

- Separate proposals for each synchrotron
  - Different values, tag names, …
- Web site access, no software interface
  - Ad-hoc, fragile software connection
- Synchrotrons (re)define formats
  but users must update data I/O code
  - N users × M synchrotrons
    = N × M converters to maintain
- Diverse access control procedures
  and information requirements
  - Access controls will never be the same,
    but procedures might be harmonised



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Alternative - using MXLIMS



With thanks to Dennis Stegmann

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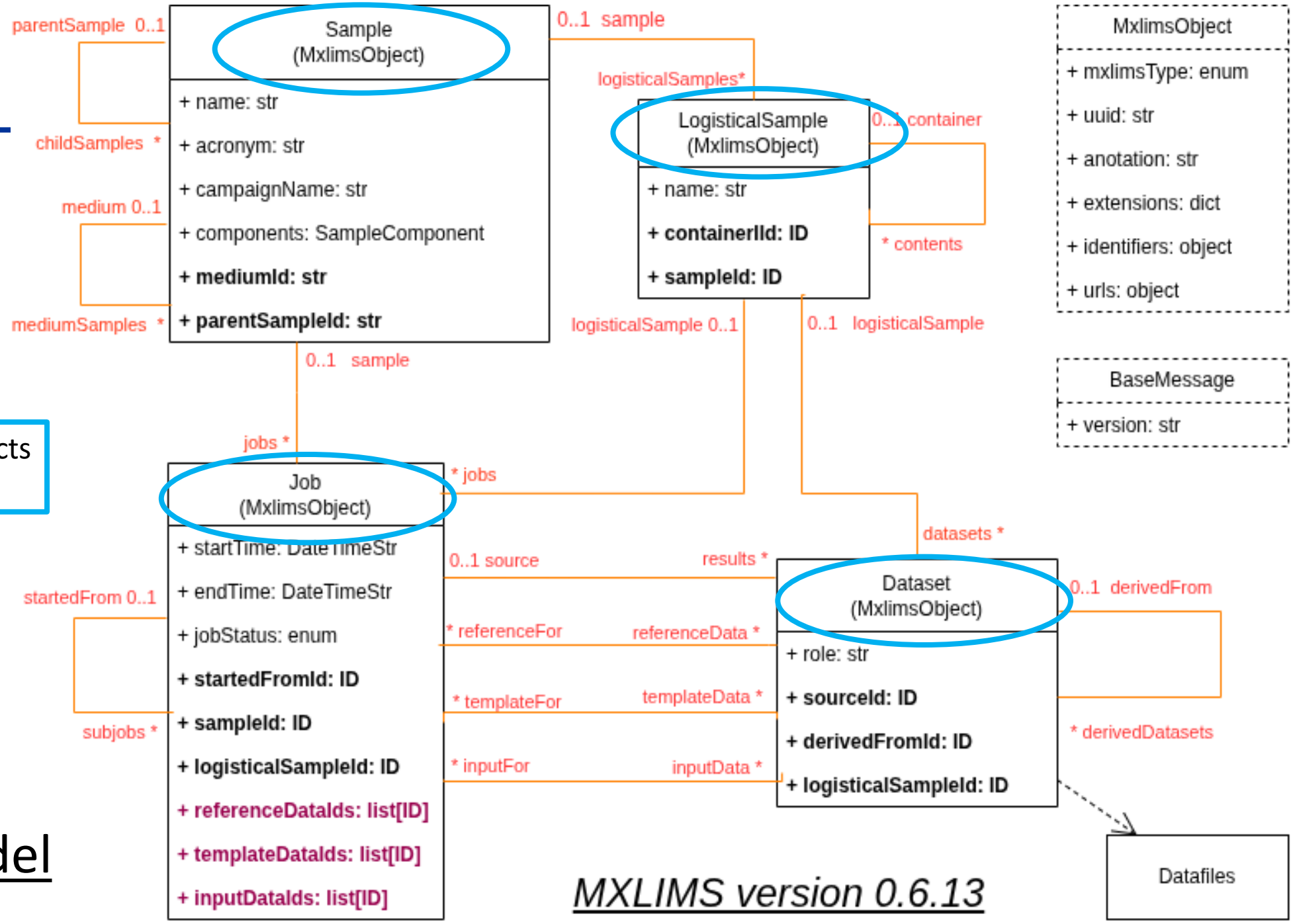
MXLIMS design

- A clearly defined standard using JSON schemas
  - JSON message files validated against the standard
  - Code generation for implementations (Pydantic, potentially noSQL databases)
- Flexibility and maintainability *(unlike ISPyB ☹)*
  - Slots for site-specific fields and identifiers, to allow extension
  - Data file versioning, so you can support multiple versions in parallel
- A simple domain-independent core
  - Metadata repository
  - Support for provenance tracking
  - Independent extension to new domains
- Reuse schemas for multiple, similar objects (e.g. diffraction plan, results)

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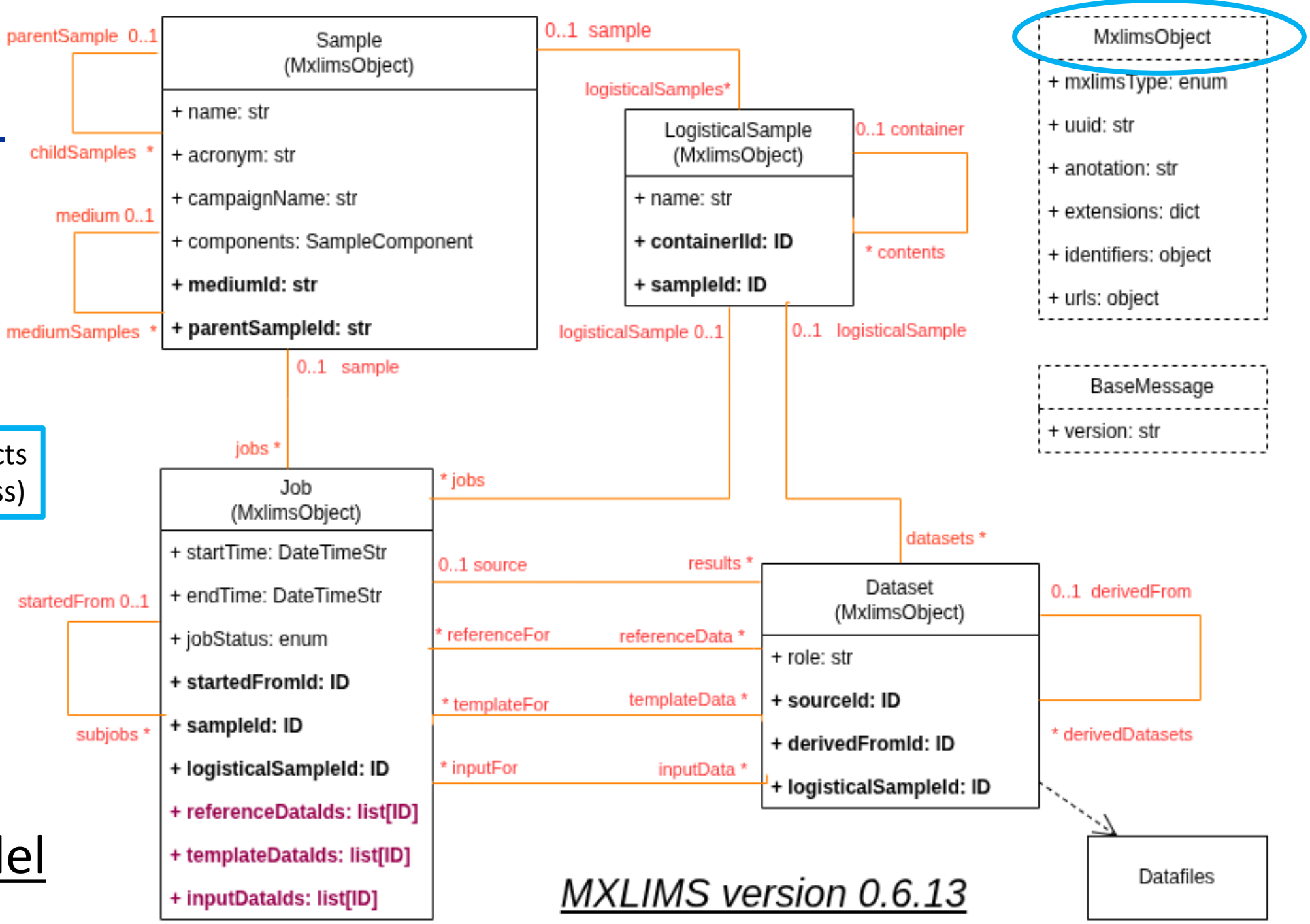
Four kinds of objects
('noSQL tables')

Core Model



MXLIMS version 0.6.13

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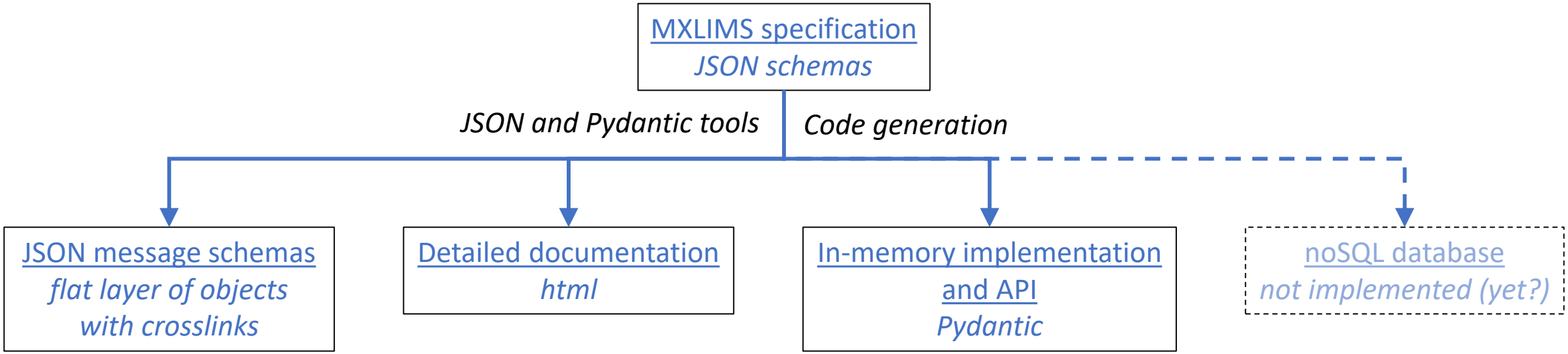
Shared by all objects (abstract superclass)

Core Model

MXLIMS version 0.6.13

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MXLIMS implementation

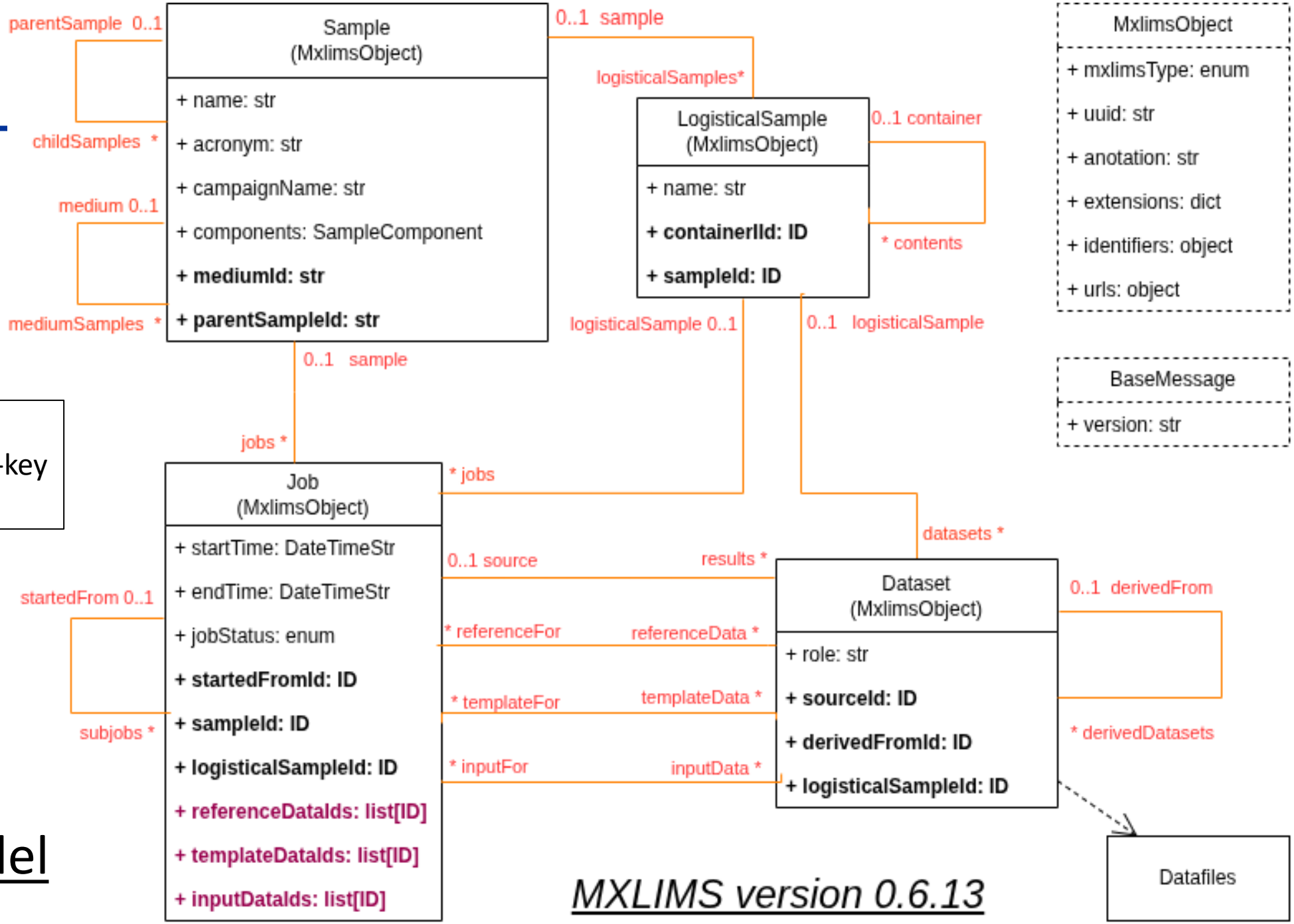


JSON supports tree structures, but objects form a web, not a tree.
Links between objects are stored as object ID pointers (foreign keys, UUIDs) also within messages.

Link handling and link type checking differs between messages, API, and different implementations.

Code generation is used to adapt the basic specification to each case.

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API-only links (in red) supported by foreign-key attributes **(in bold)**

Core Model

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Model data - examples

MxExperiment (Job)
+ experimentStrategy: str
+ expectedResolution: float
+ expectedUnitCell: UnitCell
+ priority: int
+ radiationSensitivity: float
+ selectedUnitCell: UnitCell

MxProcessing (Job)
+ programName: str
+ programVersion: str

ReflectionSet (Dataset)
+ wavelengths: List[float]
+ anisotropicDiffraction: bool
+ binningMode: str
+ numberBins: int
+ path: str
+ fileName: str
+ spaceGroupName: str
+ refinedUnitCell: UnitCell
+ operationalResolution: float
+ diffractionLimitsEstimated: Tensor
+ reflectionStatisticsOverall: ReflectionStatistics
+ reflectionStatisticsShells: List[ReflectionStatistics]

MacromoleculeSample (Sample)
+ name: str
+ acronym: str
+ campaignName: str
+ components: List[SampleComponent]

CollectionSweep (Dataset)
+ sweepType: str
+ energy: float
+ exposureTime: float
+ imageWidth: float
+ meshRange: [float, float]
+ numberImages: int
+ path: str
+ fileNameTemplate: str

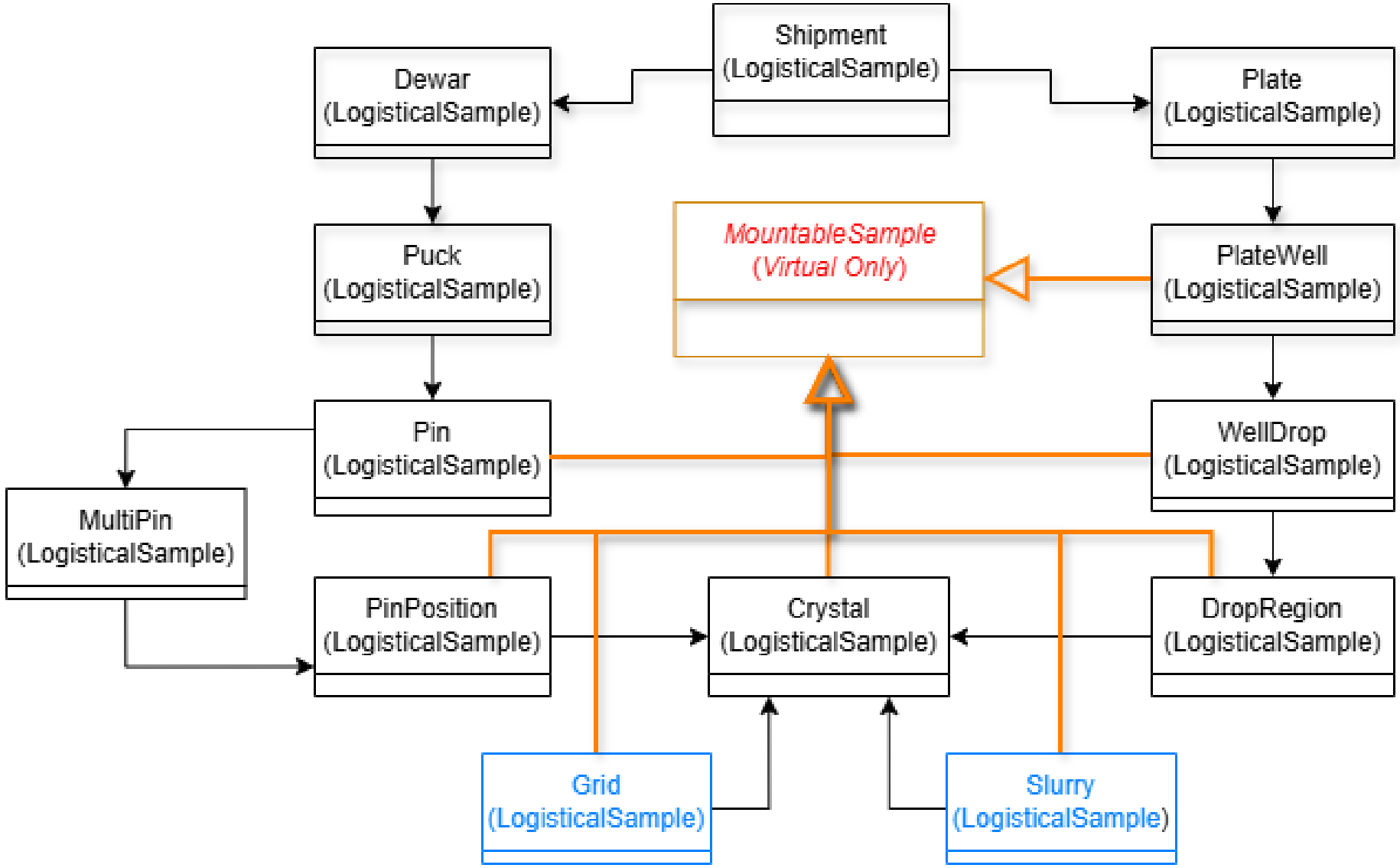
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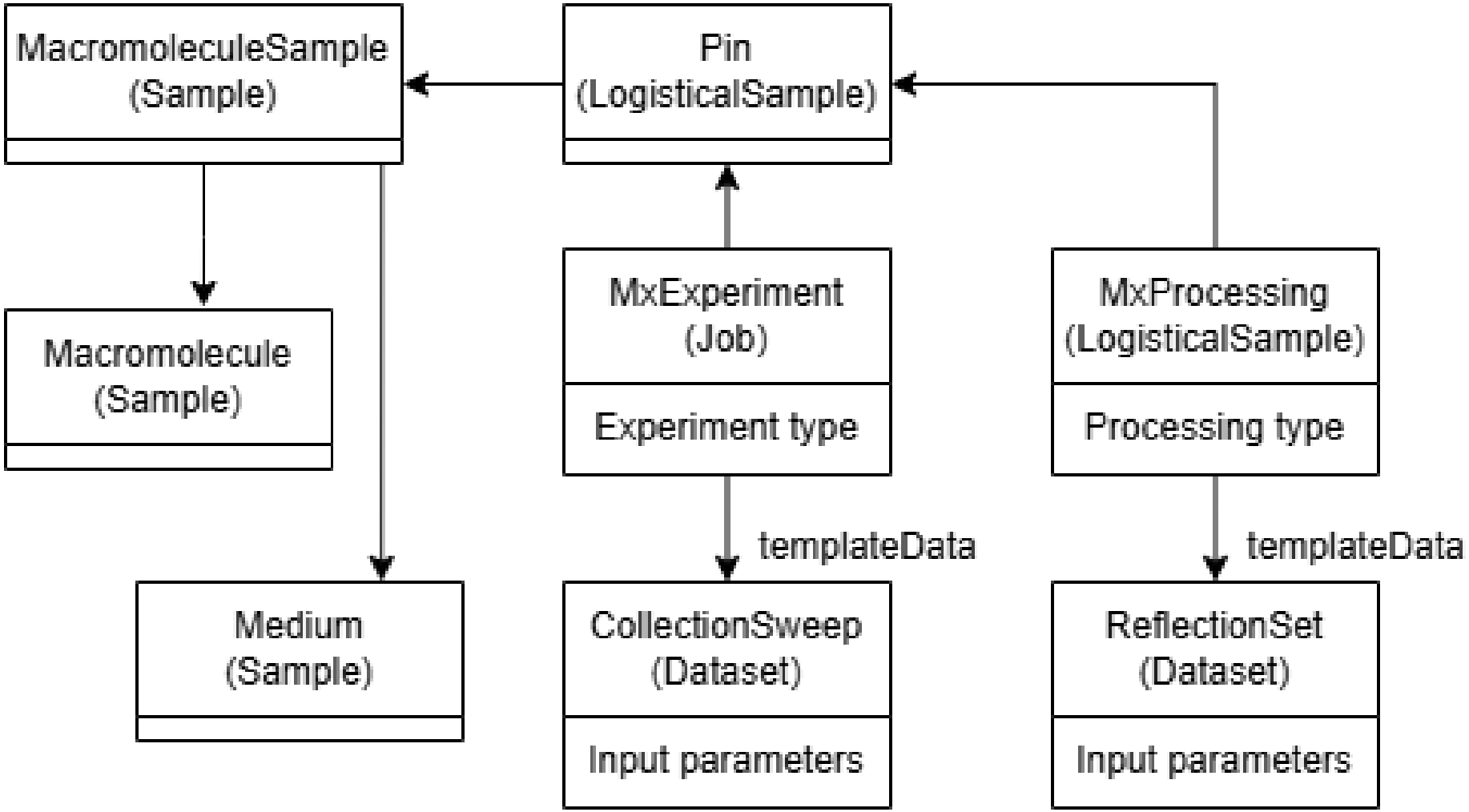
Logistical Samples

- ‘Mountable samples’ (not a real class) are samples that can be used to run an experiment on.
- Grids and slurries are not currently modeled, but would fit in as samples for SSX or XFEL.
- Crystal objects are only generated as needed. In grids, slurries, multi-crystal wells , or lipid cubic phase, crystals cannot be identified before the experiment



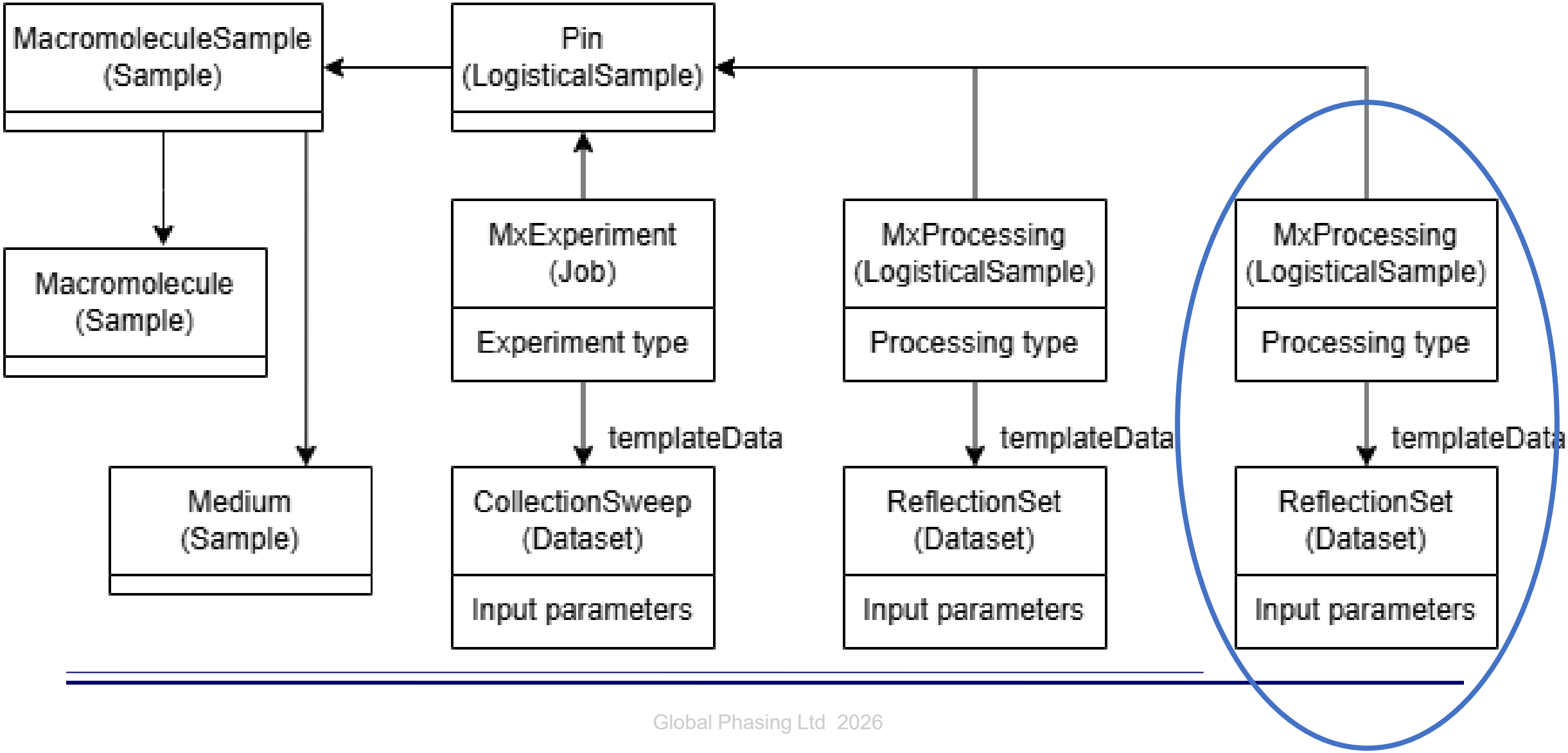
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Experiment input



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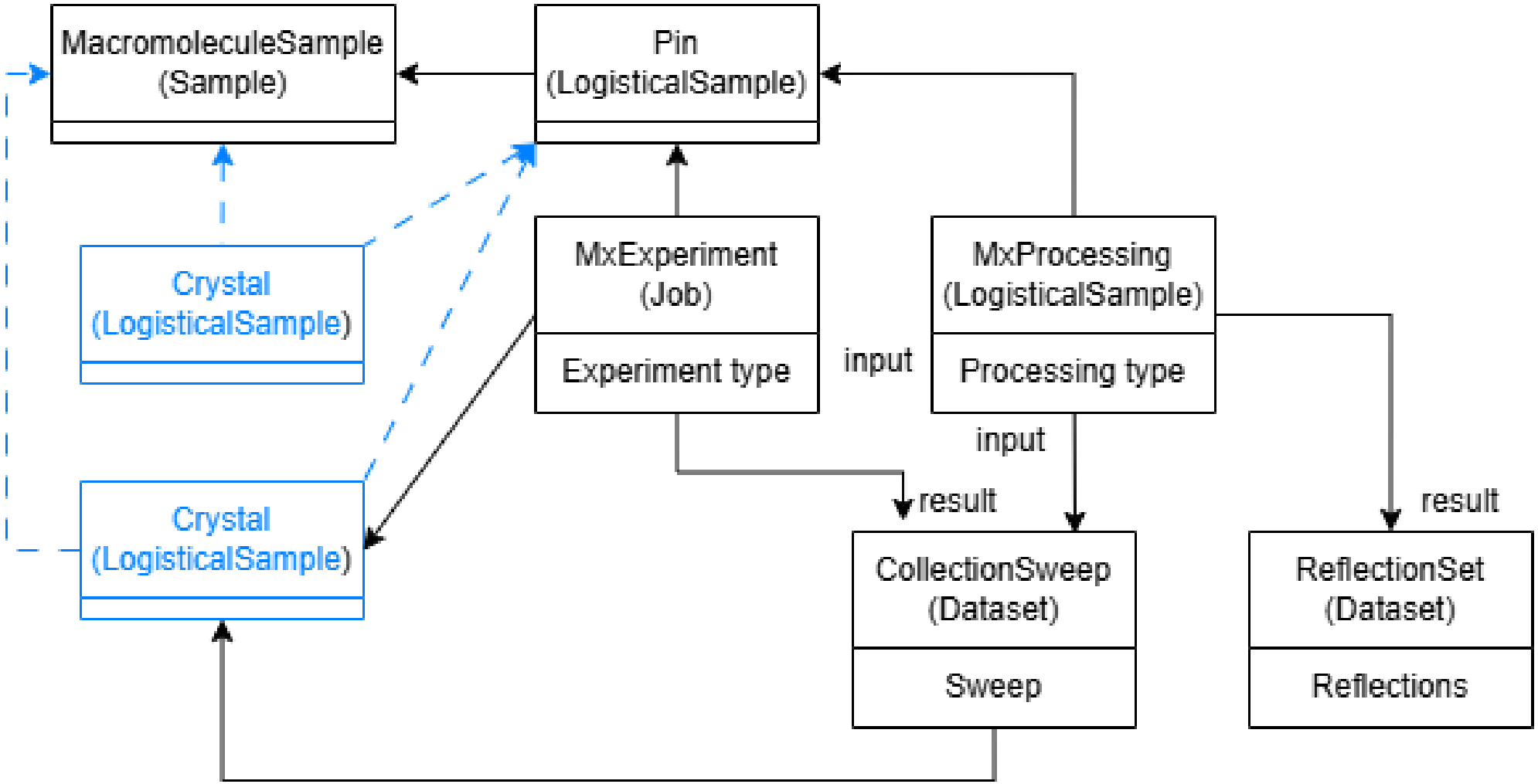
Experiment input – multiple processing



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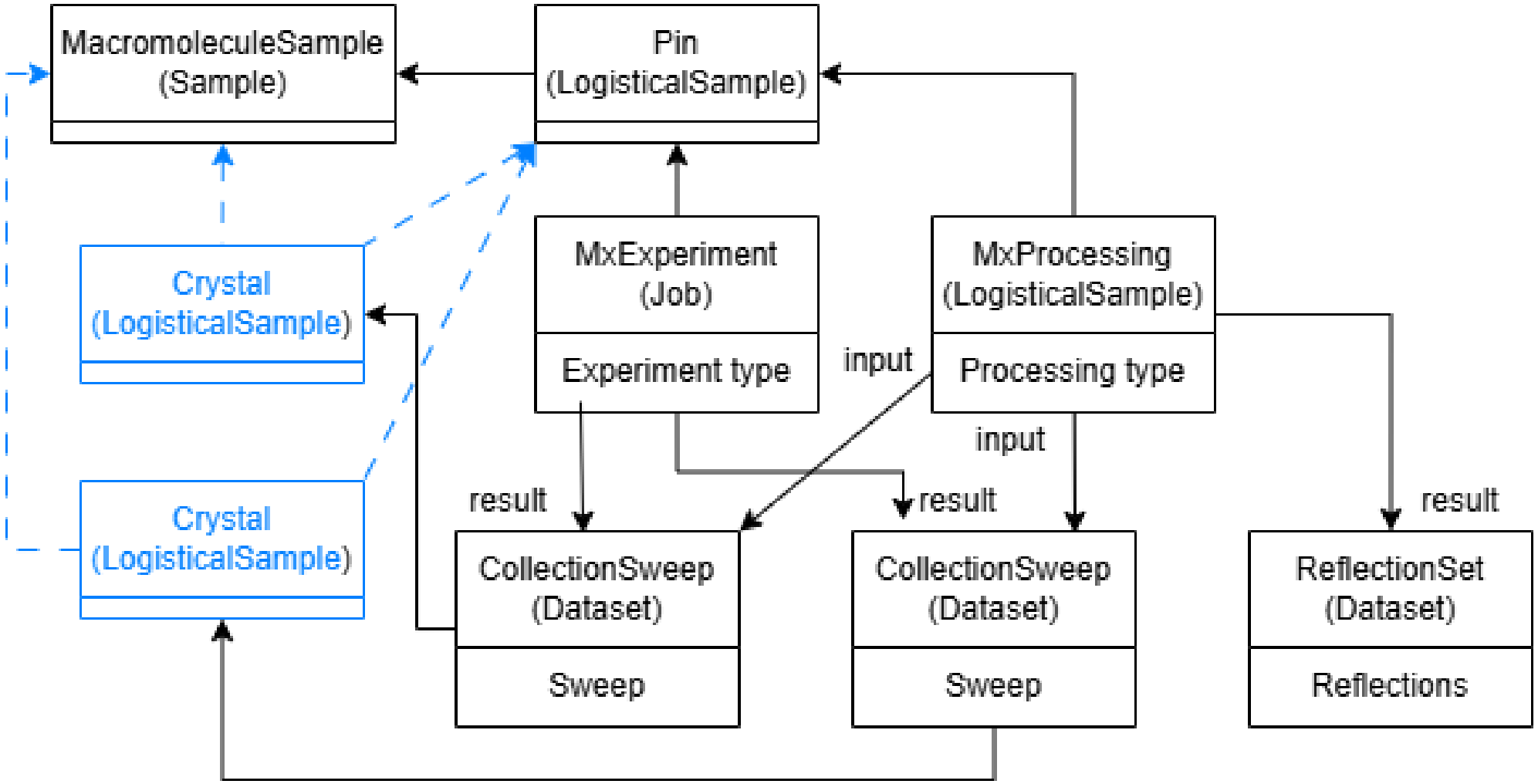
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Experiment results



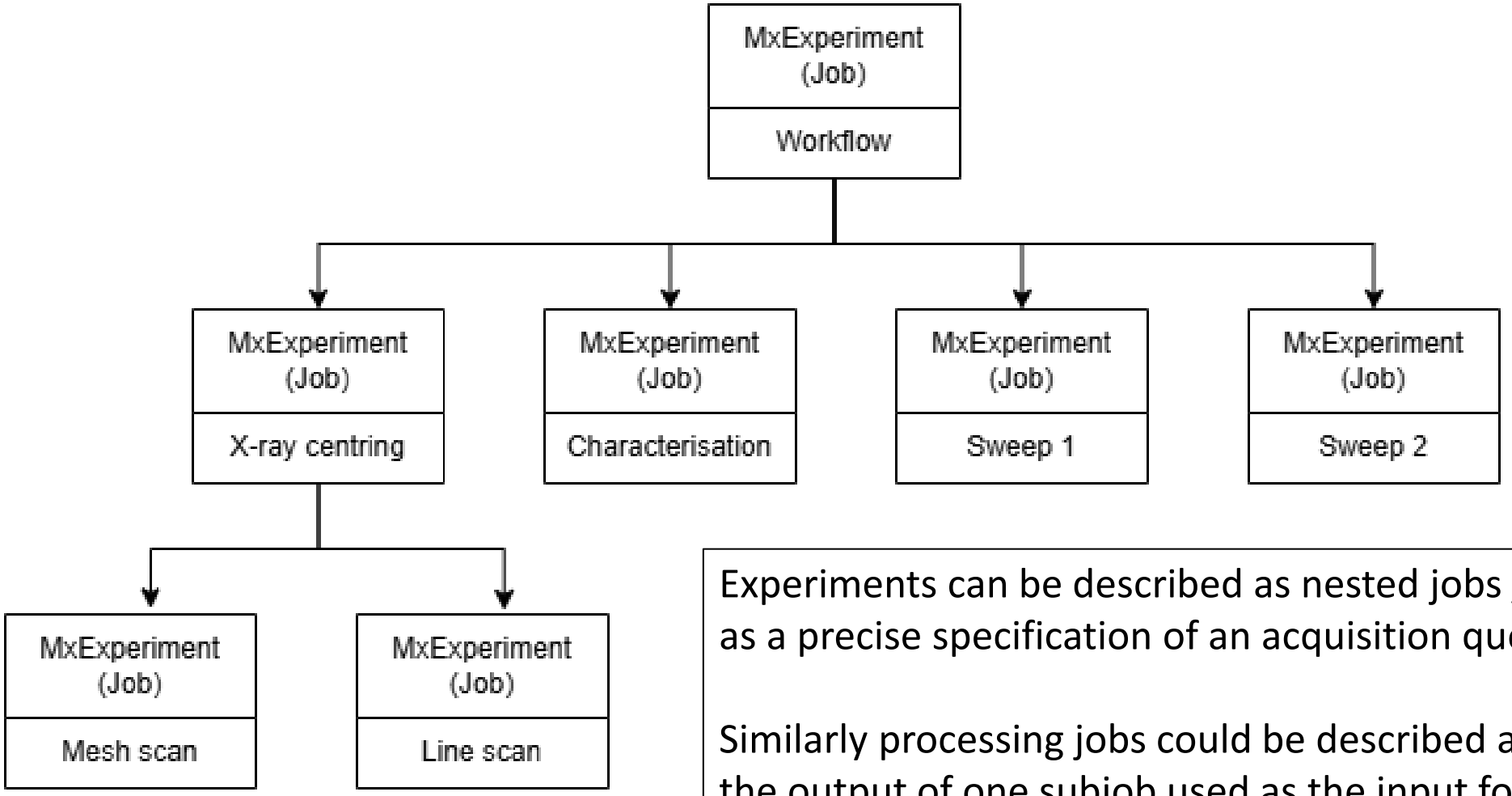
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Multi-crystal multi-sweep experiment



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Nested jobs / subjobs



Experiments can be described as nested jobs / subjobs, e.g. as a precise specification of an acquisition queue.

Similarly processing jobs could be described as nested, with the output of one subjob used as the input for others.

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Getting organised

- MXLIMS is not a private project, but a nascent community standard
- As new participants join, the project will be reorganised:
  - Shared, public repositories
  - Procedures for accepting changes, making new versions etc.
  - Governance by stakeholders

- MXLIMS is ready for you to join in!

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Acknowledgements

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- For work on integration, synchrotron mapping and testing and making the MXLIMS model, particular thanks to Guilherme de Freitas, James Hall, Jose Brandao-Neto and Karl Levik (Diamond), Daniele de Sanctis, Didier Nurizzo, Marcus Oscarsson, Olof Svensson, and Yan Walesch (ESRF), Leigh Carter, Clemens Vonrhein and Peter Keller (Global Phasing), Ed Daniel (IceBear), Ezequiel Panepucci (MAX IV), Dennis Stegmann and May Sharpe (SLS), Martin Savko (SOLEIL), and Gustavo Lima (Astex)