



U.S. ARMY COMBAT CAPABILITIES DEVELOPMENT COMMAND ARMY RESEARCH LABORATORY

HTMDEC Data Science Overview

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ASPIRATIONS



Holy grail:

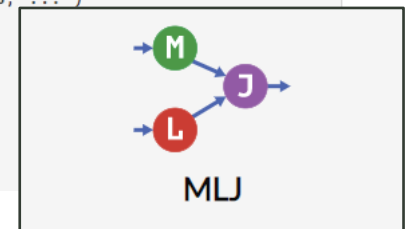
Enter research problem → suitable analyses and workflows are suggested
→ robot executes

Anybody can do it:

- Compose research workflow from components for data capture, analysis, and **decision** pipelines
- Low-code, no-code approach
- Lower barrier to program planning and execution
- **High reusability**

To list *all* models available in MLJ's `model registry` do `models()`. Listing the models compatible with the present data:

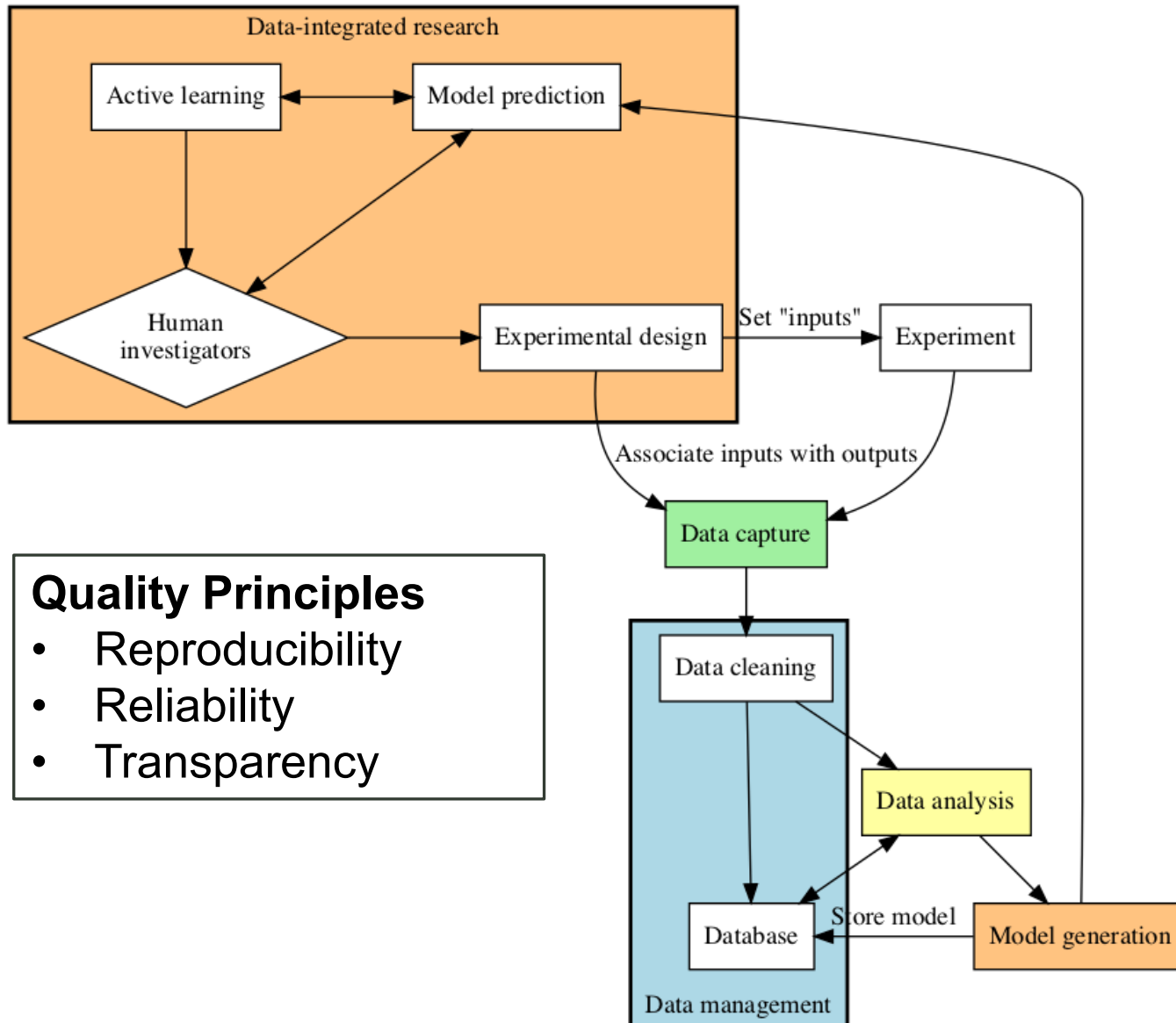
```
julia> models(matching(X,y))
42-element Array{NamedTuple{(:name, :package_name, :is_supervised, :docstring, :hyperparameter_
 (name = AdaBoostClassifier, package_name = ScikitLearn, ... )
 (name = AdaBoostStumpClassifier, package_name = DecisionTree, ... )
 (name = BaggingClassifier, package_name = ScikitLearn, ... )
 (name = BayesianLDA, package_name = MultivariateStats, ... )
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 (name = BayesianQDA, package_name = ScikitLearn, ... )
 (name = BayesianSubspaceLDA, package_name = MultivariateStats, ... )
 (name = ConstantClassifier, package_name = MLJModels, ... )
 (name = DecisionTreeClassifier, package_name = DecisionTree, ... )
 (name = DeterministicConstantClassifier, package_name = MLJModels, ... )
 :
 (name = RidgeCVCClassifier, package_name = ScikitLearn, ... )
 (name = RidgeClassifier, package_name = ScikitLearn, ... )
 (name = SGDCClassifier, package_name = ScikitLearn, ... )
 (name = SVC, package_name = LIBSVM, ... )
 (name = SVMClassifier, package_name = ScikitLearn, ... )
 (name = SVMClassifier, package_name = ScikitLearn, ... )
```



Also see: AutoML, autoconfig, Orange Data Mining, BPMS, cookiecutter, DrWatson.jl, or Data Versioning Control frameworks

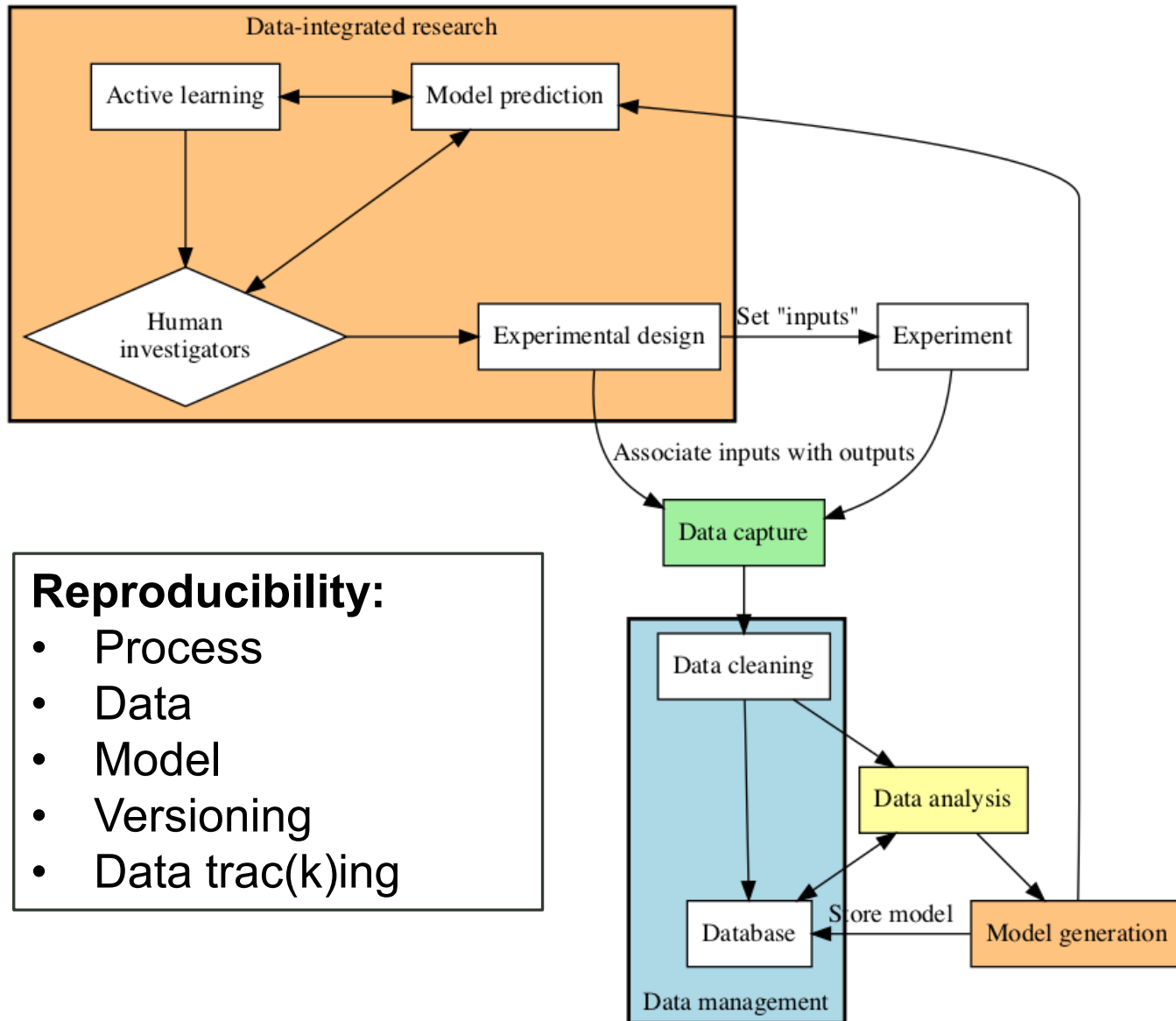


DATA INFORMED RESEARCH FLOW



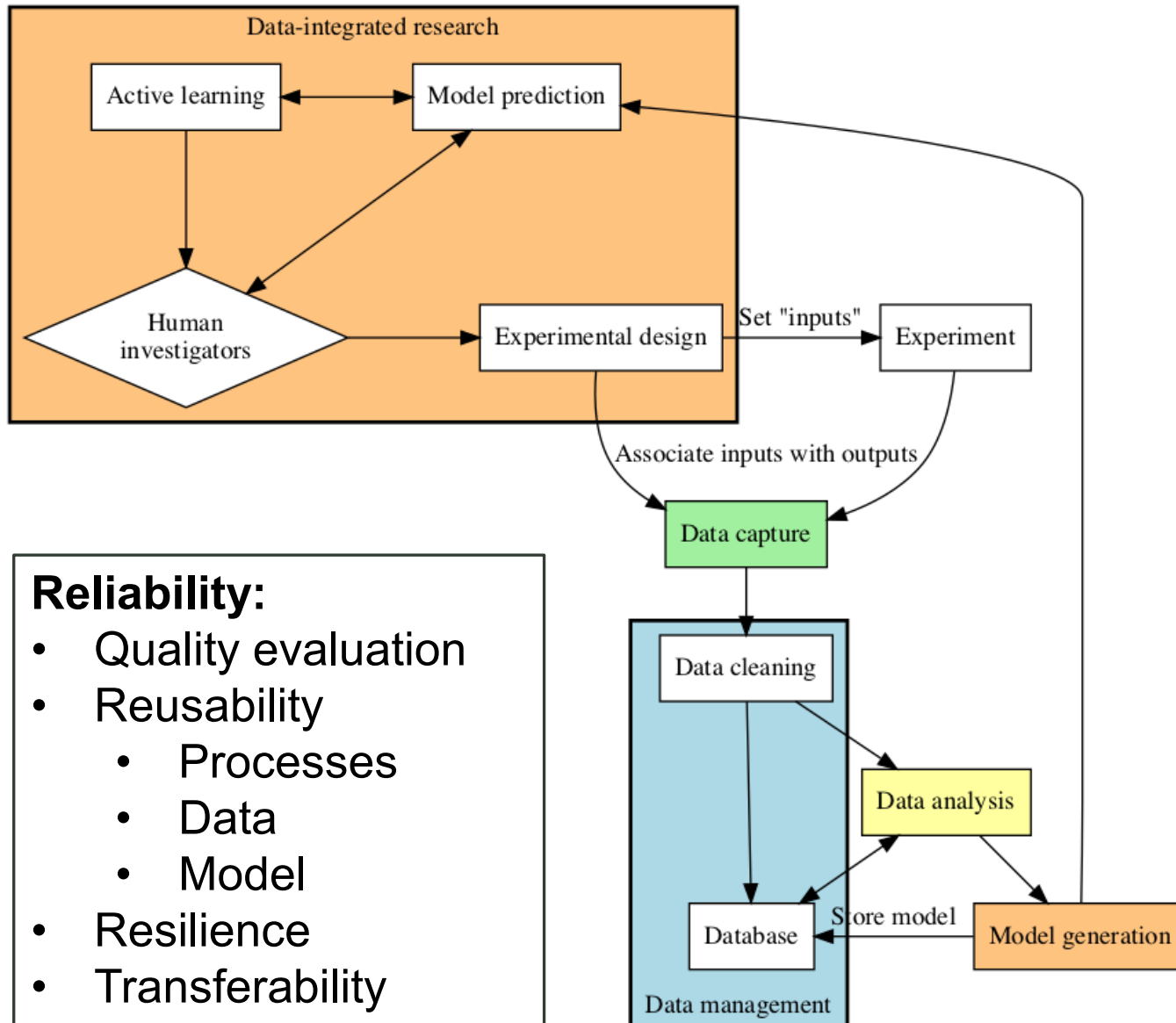


DATA INFORMED RESEARCH FLOW



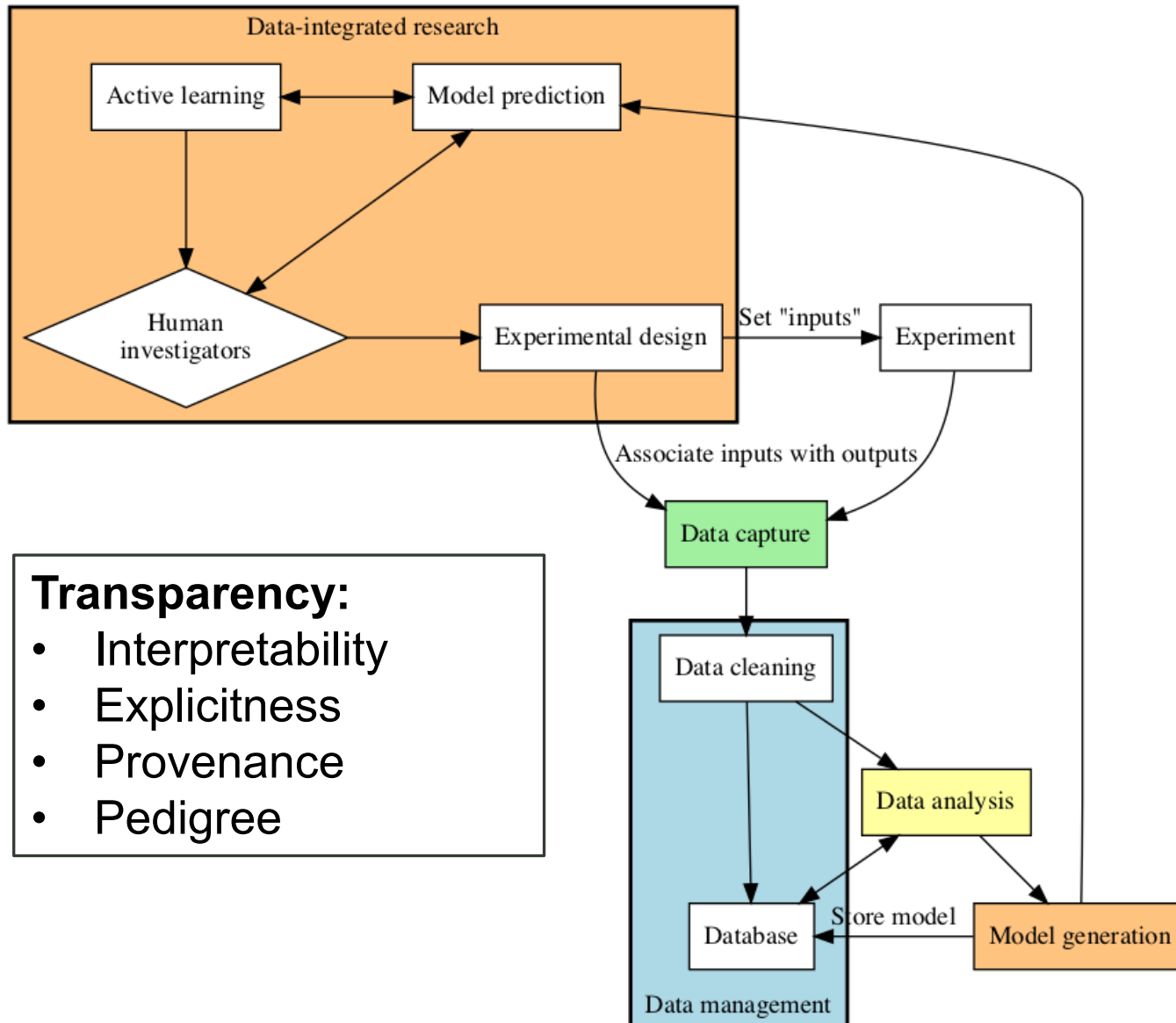


DATA INFORMED RESEARCH FLOW



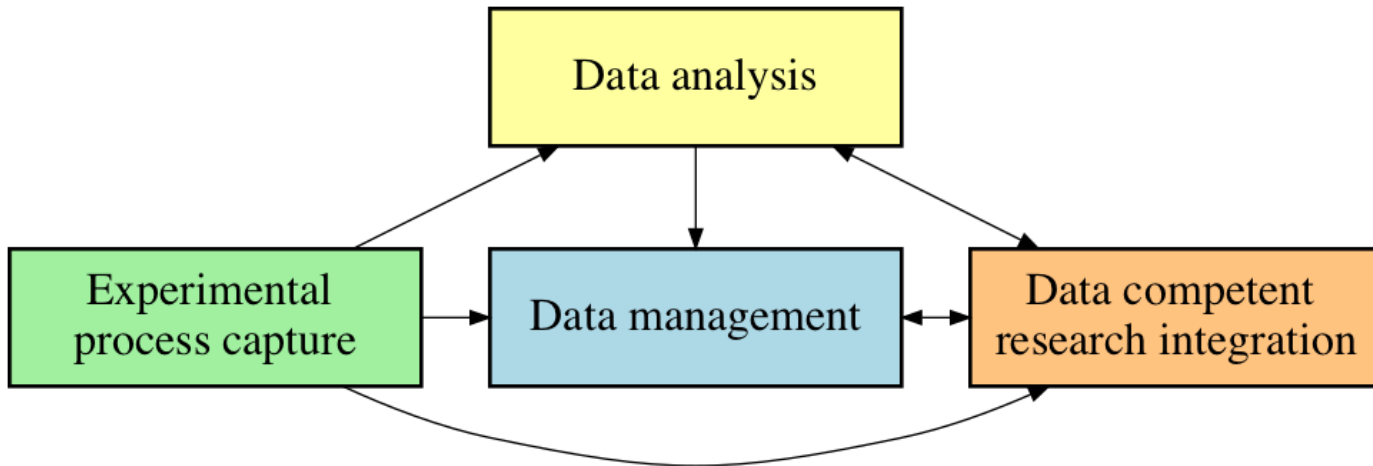


DATA INFORMED RESEARCH FLOW



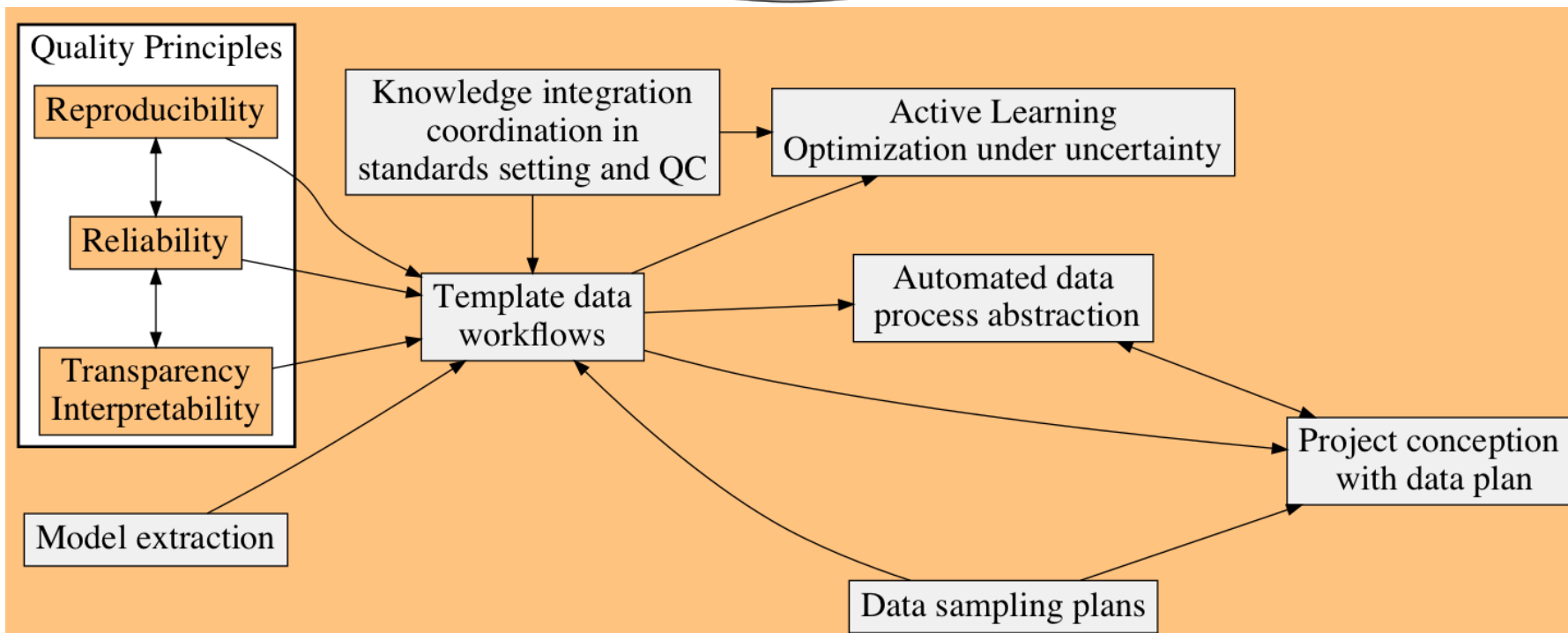
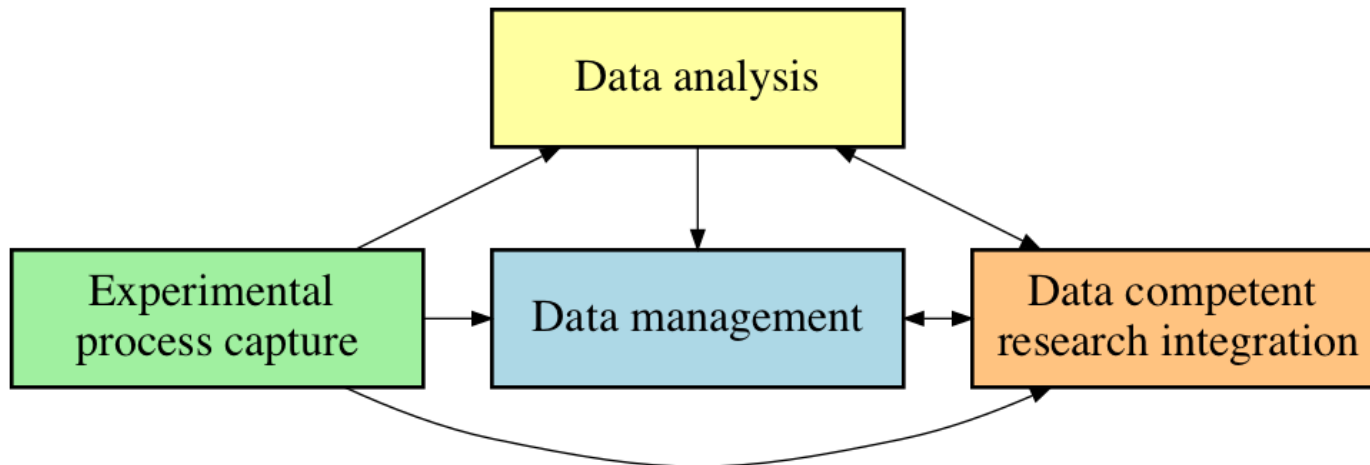


DATA INFORMED RESEARCH REQUIREMENTS



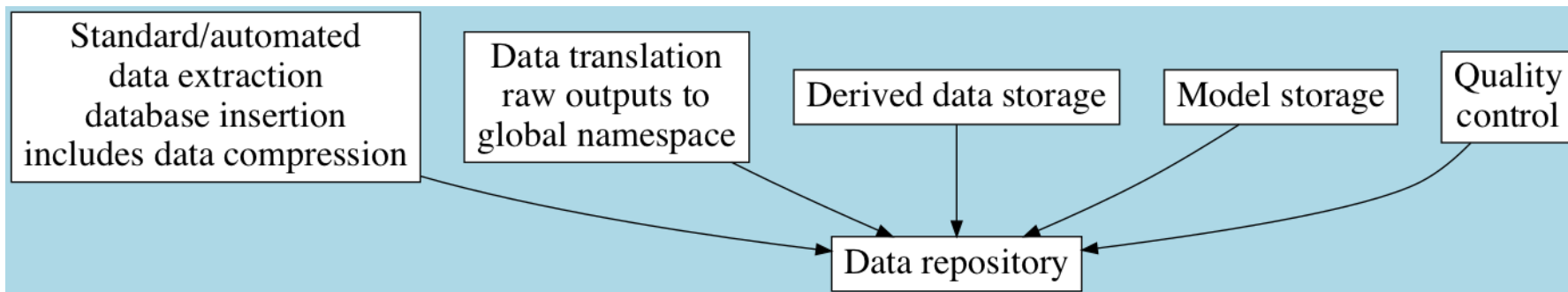
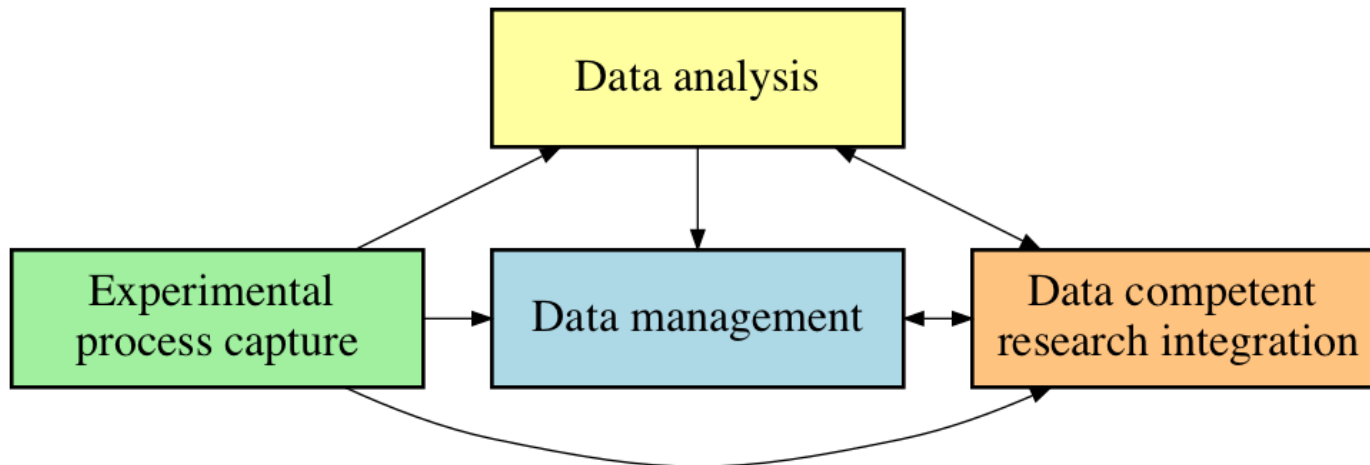


DATA COMPETENT RESEARCH INTEGRATION



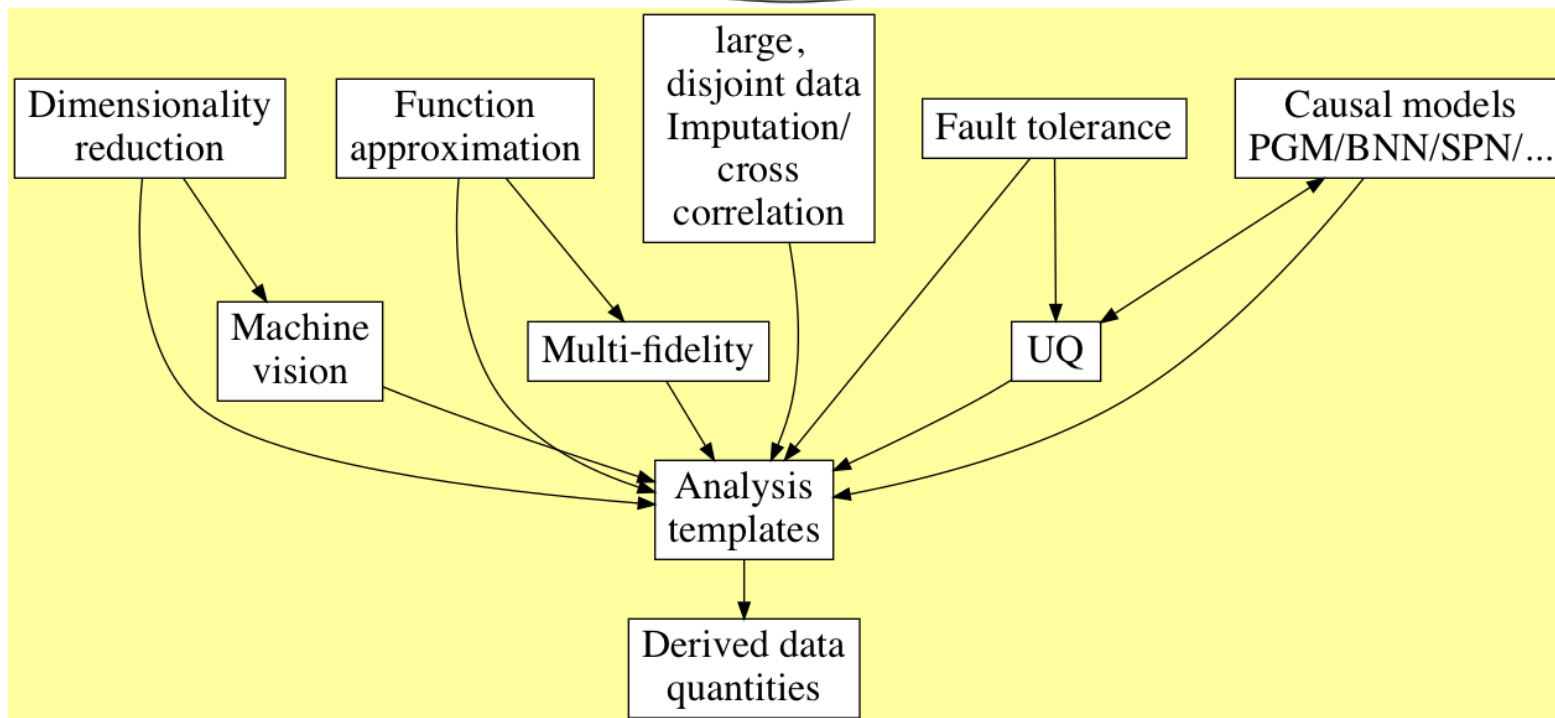
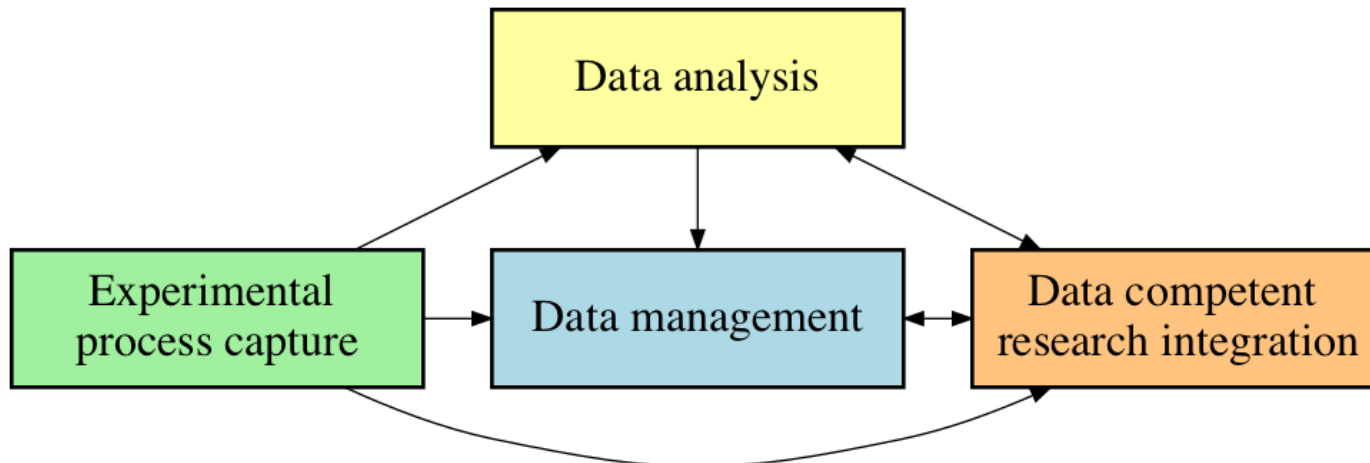


DATA MANAGEMENT COMPONENTS



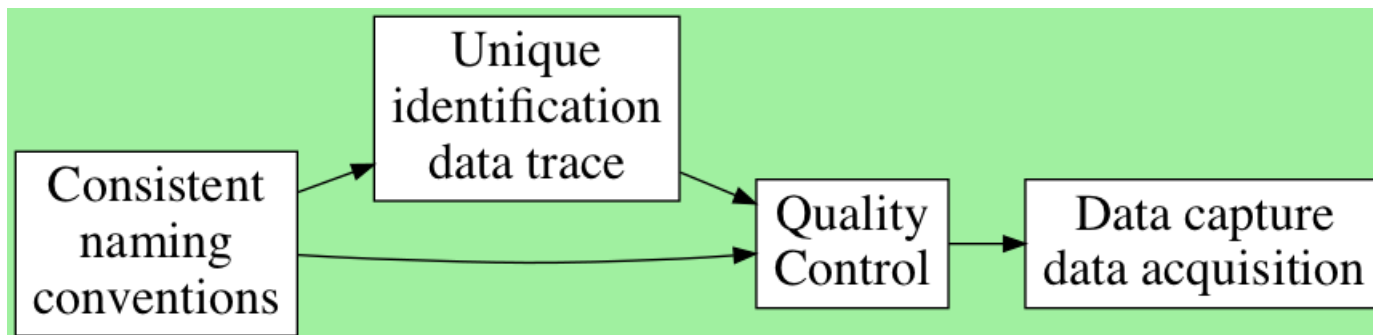
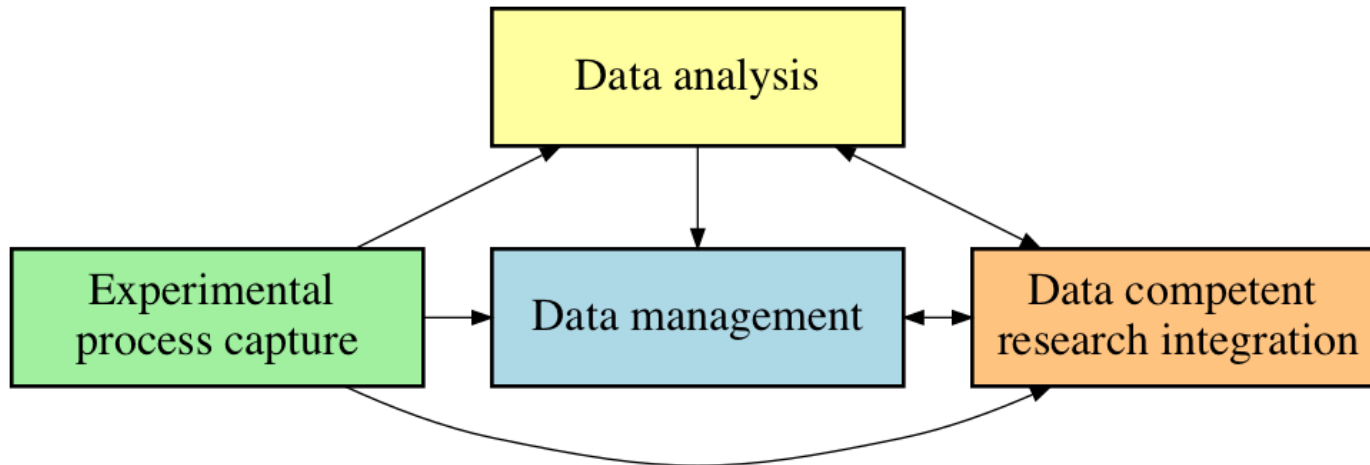


DATA ANALYSIS COMPONENTS



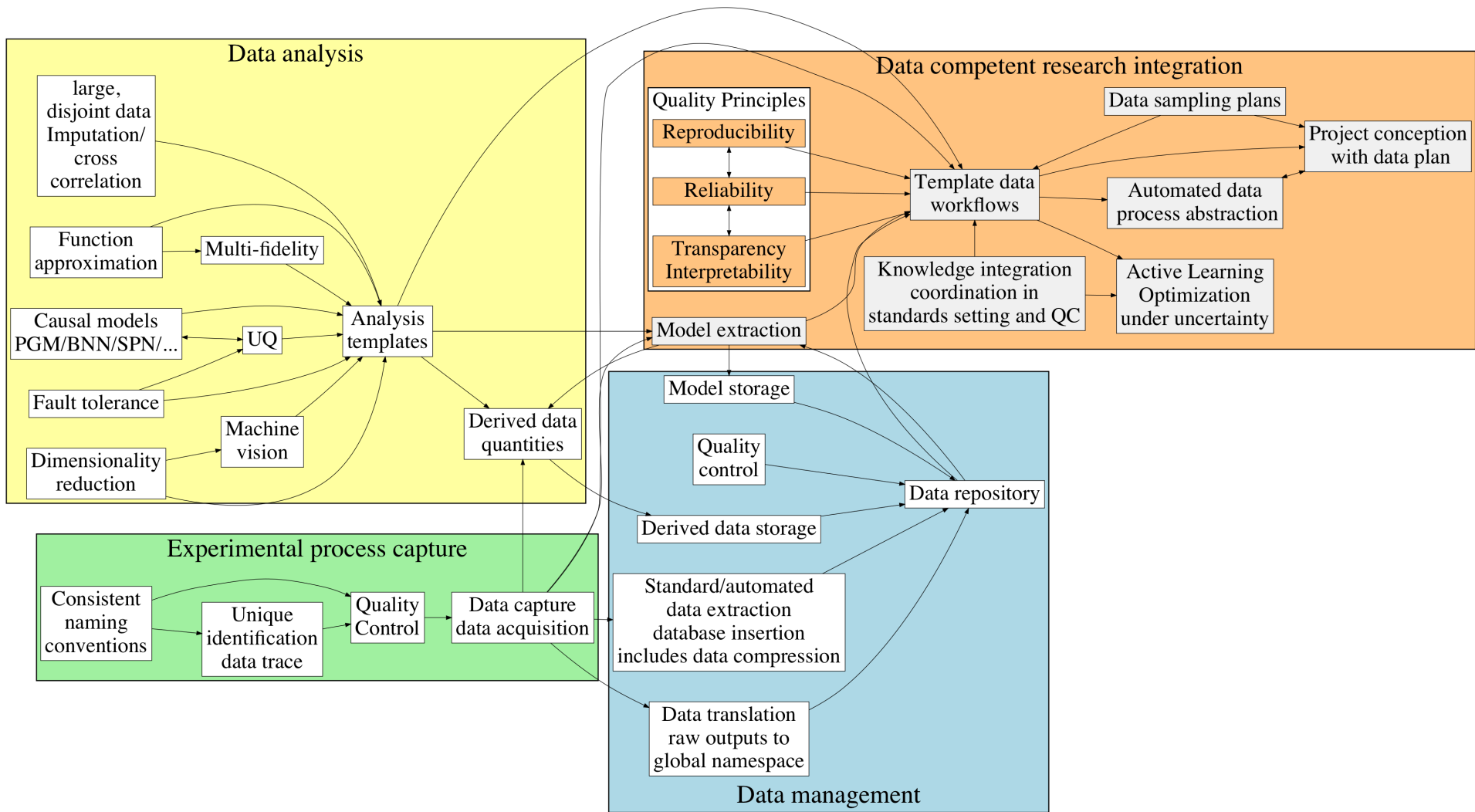


DATA CAPTURE/ACQUISITION





FULL DATA DEPENDENCY GRAPH





COMPOSABLE BUILDING BLOCKS



Dimensionality Reduction

Modeling Blocks

Process Building Blocks

Processes

SPN

VAE (CNN)

t-SNE

⋮

NN

Schema

SVM

GPR

⋮

Denoising

XRD

SEM

Tensile Testing

Hardness

Image Comparison

Data Fusion

AFM

Simulation

Printability

Ceramics AM

Metals AM

(S)PGM

⋮

Database Retrieval

Database Scouring

Data Capture

Data curation

Schema Extraction

Database Management



CHALLENGES



Reproducibility Challenges

- Data drift
- Concept drift
- UX/UI
- Equivalence problem
- User error detection

Reliability Challenges

- Interoperability
- Schema consistency
- Domain specific conventions

Transparency Challenges

- UX/automation balance
- Data/Process Visualization
- Documentation overhead
- Process development
- Findability/Access control/Information security

- User error mitigation
- Problem-specific UQ
- Applicability assessment



Backup Slides