Optimization in Analytical and Scientific Workflows

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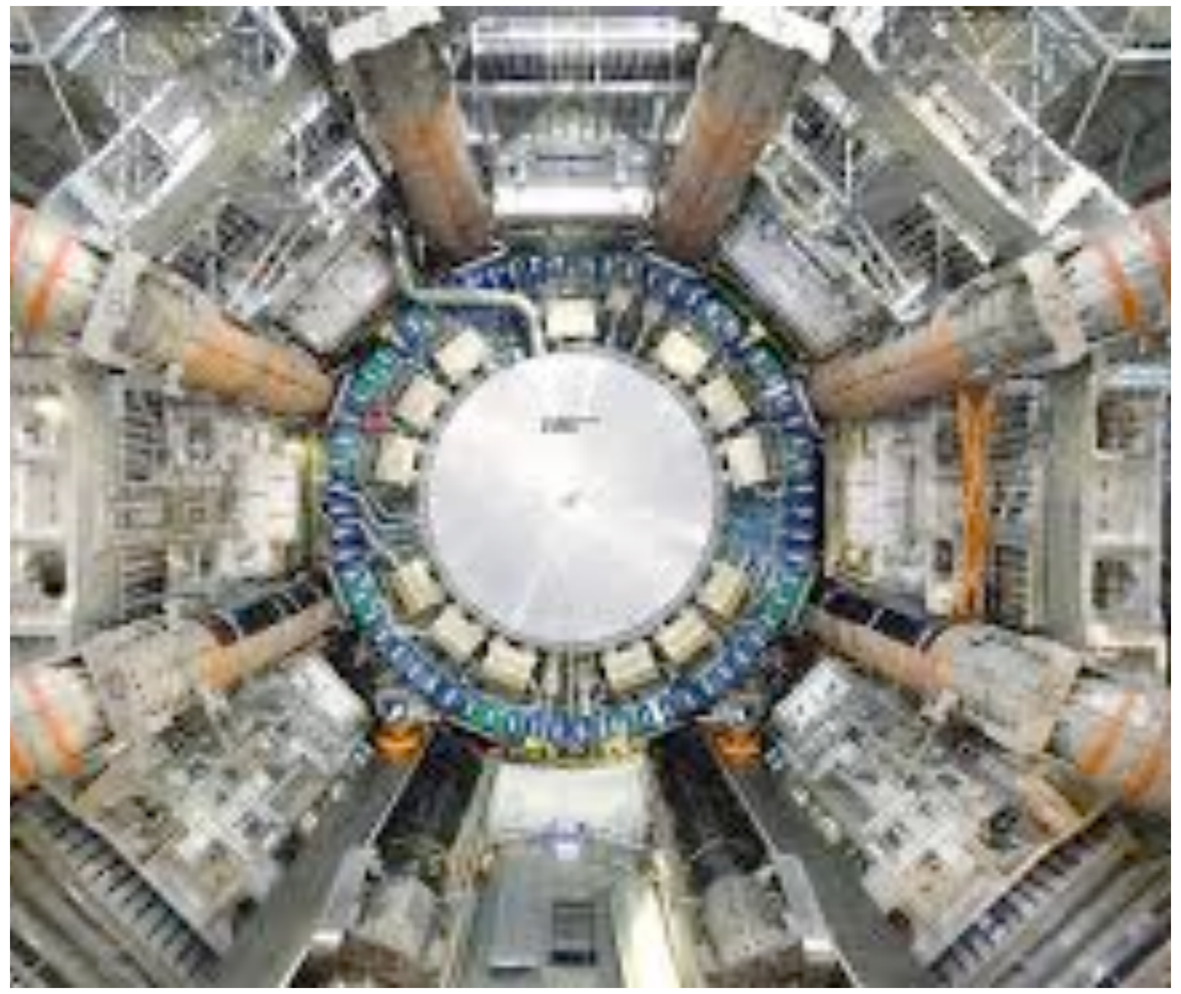
What are the common key elements of scientific discovery ?

Omics

Physics



Astrophysics

Social Science

Data-intensive Science

Scientific discovery relies on workflows and data

Generic scientific worflow

A scientific worflow is a process for accomplishing a scientific objective, typically expressed as a series of tasks related to hypothesis testing, physical experimentations and measurements that produce data

Scientific Discovery relies on workflows and data

Generic scientific worflow

A scientific worflow is a process for accomplishing a scientific objective, typically expressed as a series of tasks related to hypothesis testing, physical experimentations and measurements that **produce data**, **which can be further analyzed via multiple computational steps.**

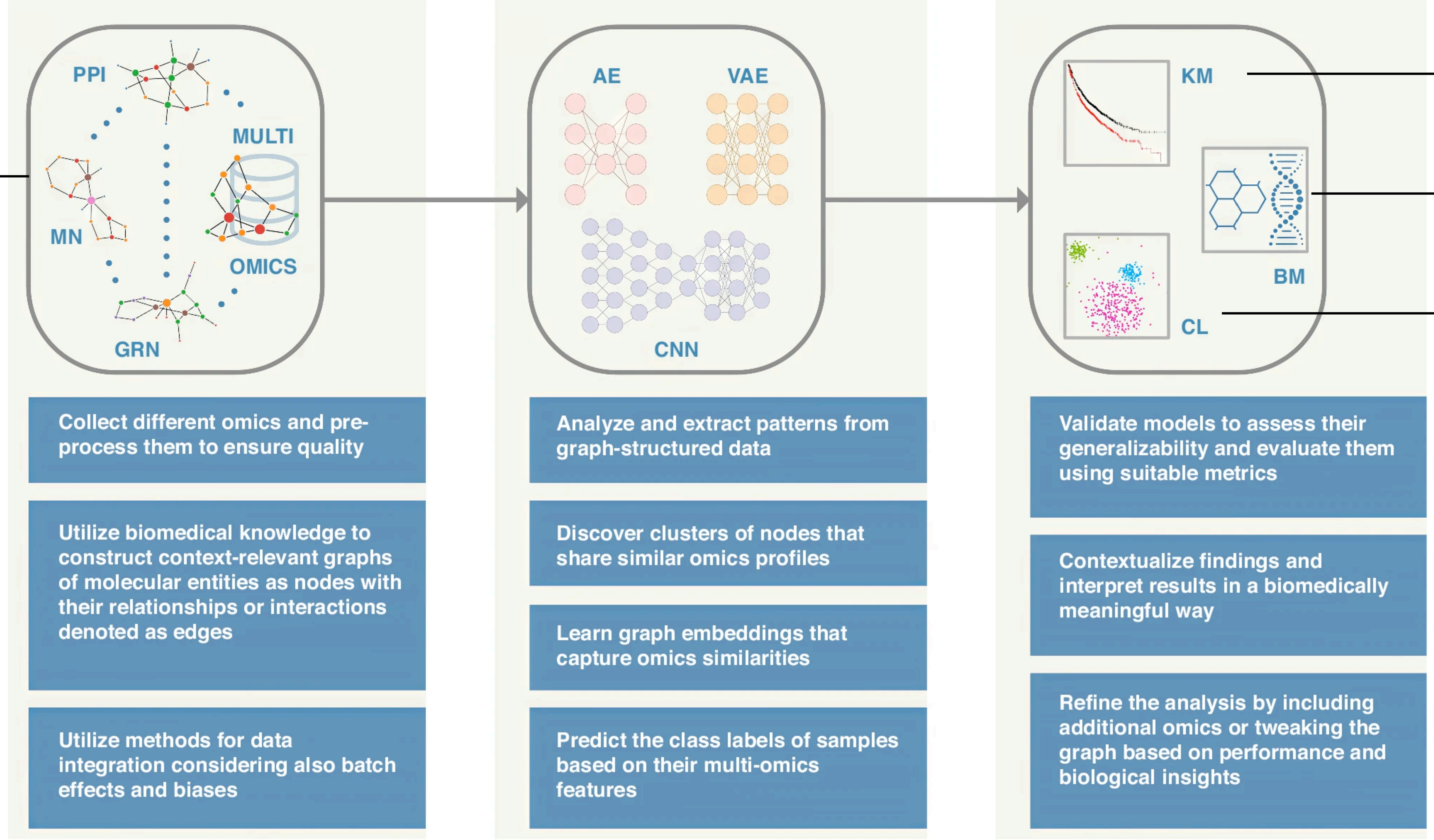
→ ***refered as analytic worflows or data science pipelines***

Scientific Discovery relies on workflows and data

Examples in Large-Scale Multi-Omics Studies

Input: Massive data | **Machine learning** | **Output: biomedical outcomes**

genomics
epigenomics
proteomics
transcriptomics
metagenomics
metabolomics
protein-protein interaction
metabolic networks
gene regulatory networks

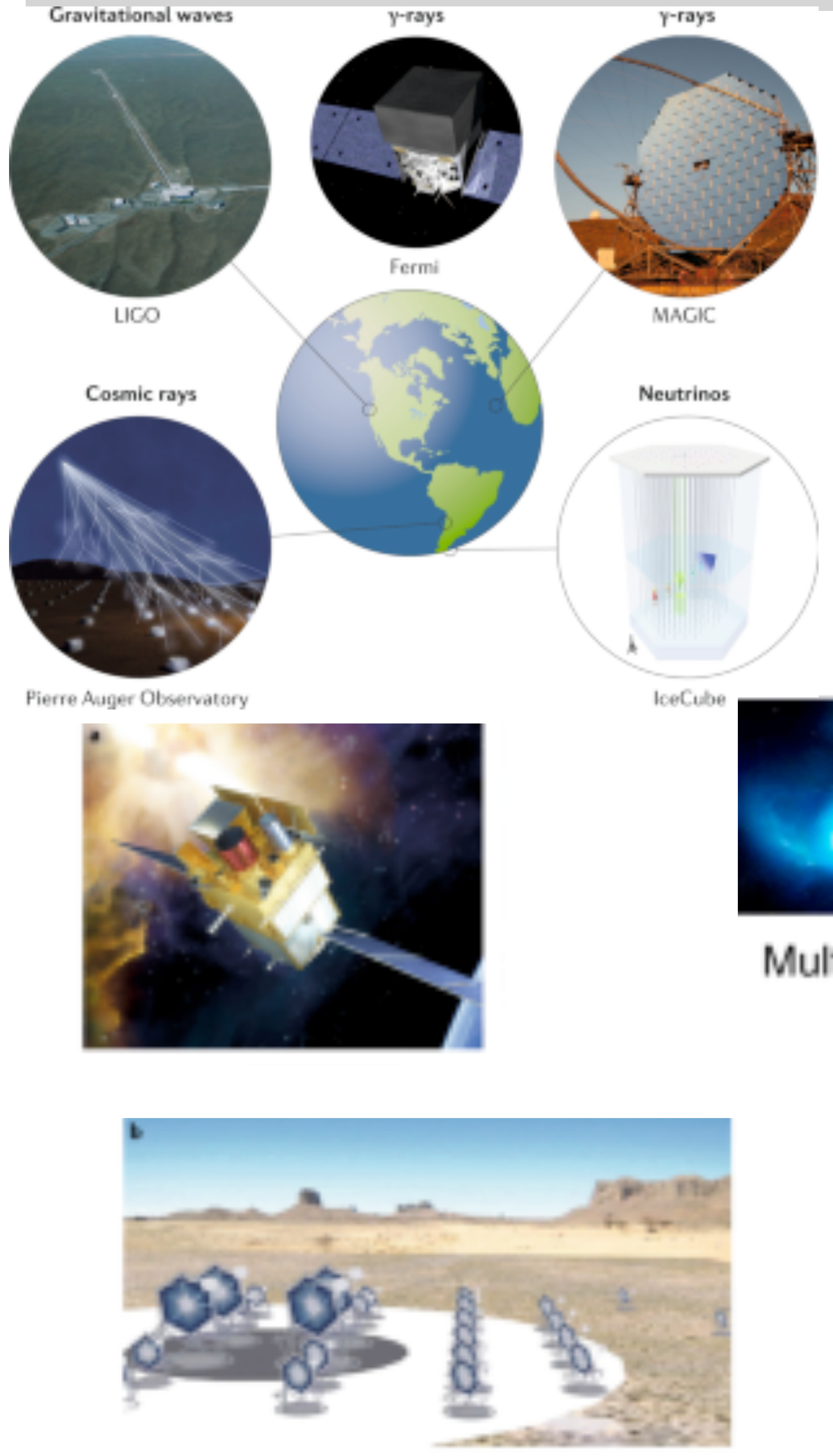


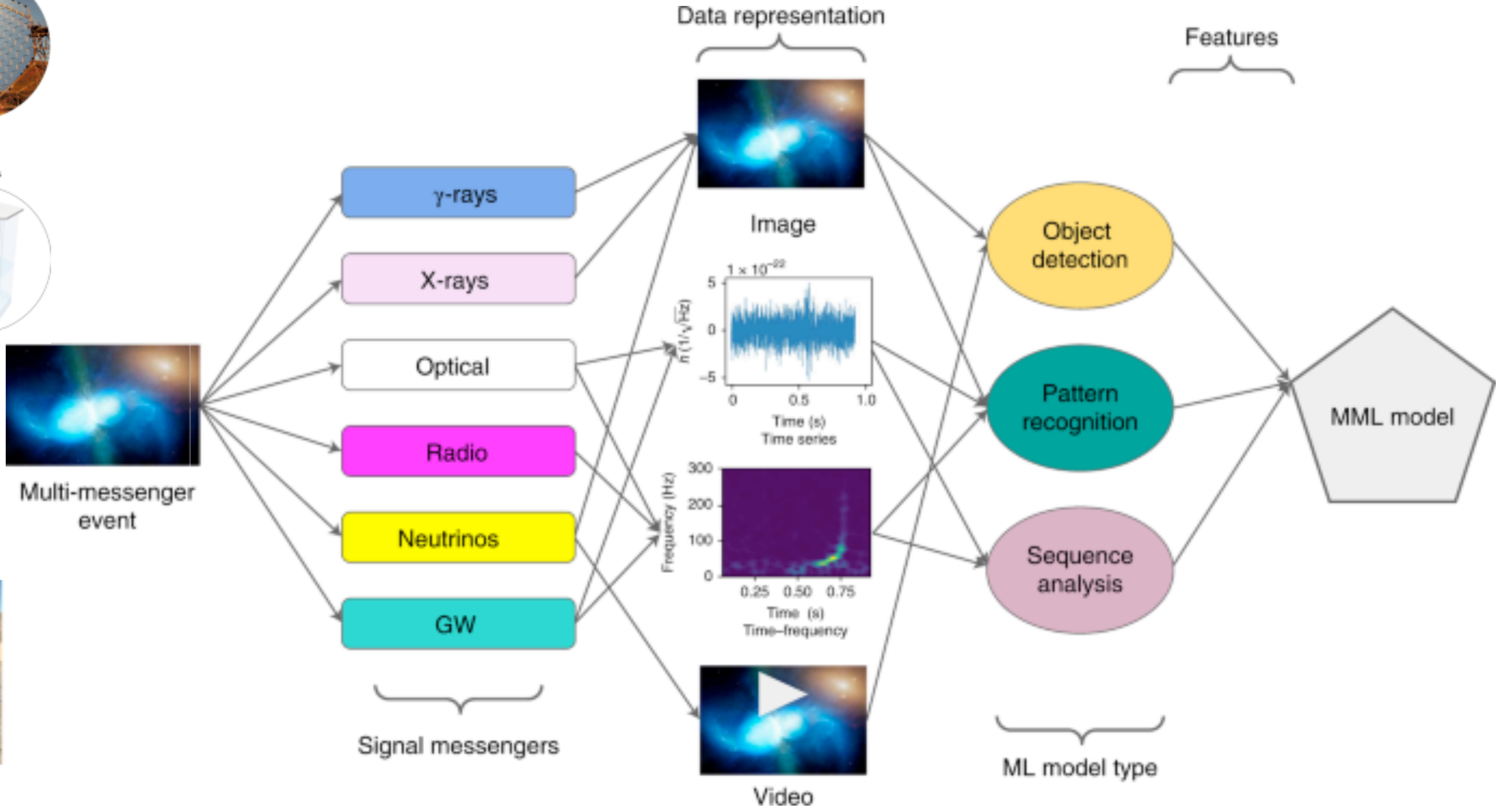
predict patient survival
identify potential biomarker candidates
patient clustering

Source: Valous, N.A., Popp, F., Zörnig, I. *et al.* Graph machine learning for integrated multi-omics analysis. *Br J Cancer* **131**, 205–211 (2024). https://doi.org/10.1038/s41416-024-02706-7
Zheng, Y., Liu, Y., Yang, J. *et al.* Multi-omics data integration using ratio-based quantitative profiling with Quartet reference materials. *Nat Biotechnol* **42**, 1133–1149 (2024). https://doi.org/10.1038/s41587-023-01934-1

Examples in Multimodal Astrophysics

Data Acquisition	Data encoding	Machine learning	Output: Astrophysical event detection





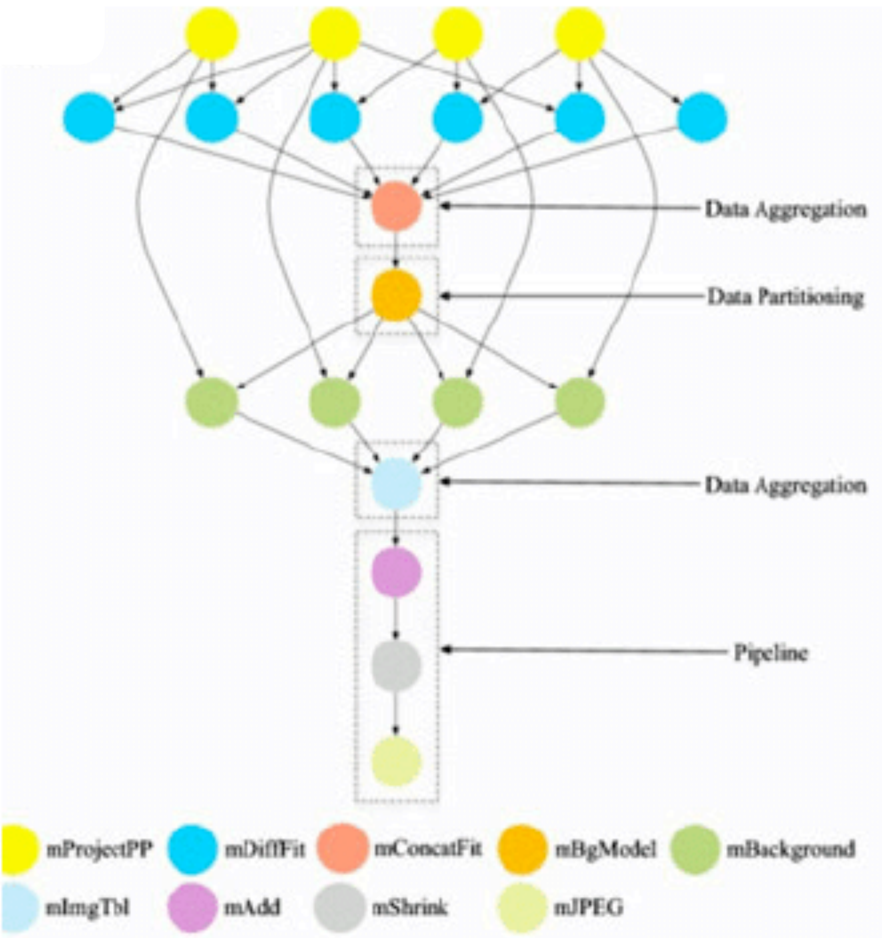
Source: Cuoco, E., Patricelli, B., Iess, A. *et al.* Computational challenges for multimodal astrophysics. *Nat Comput Sci* **2**, 479–485 (2022). https://doi.org/10.1038/s43588-022-00288-z
Mészáros, P., Fox, D.B., Hanna, C. *et al.* Multi-messenger astrophysics. *Nat Rev Phys* **1**, 585–599 (2019). https://doi.org/10.1038/s42254-019-0101-z

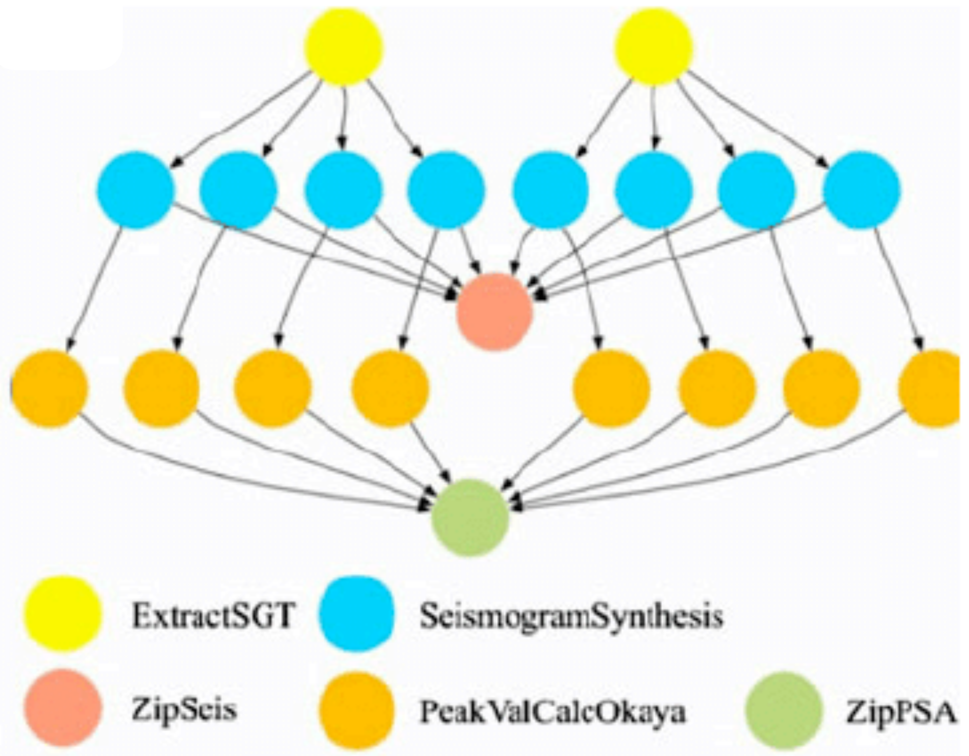
Many other examples of analytical workflows…

Pegasus

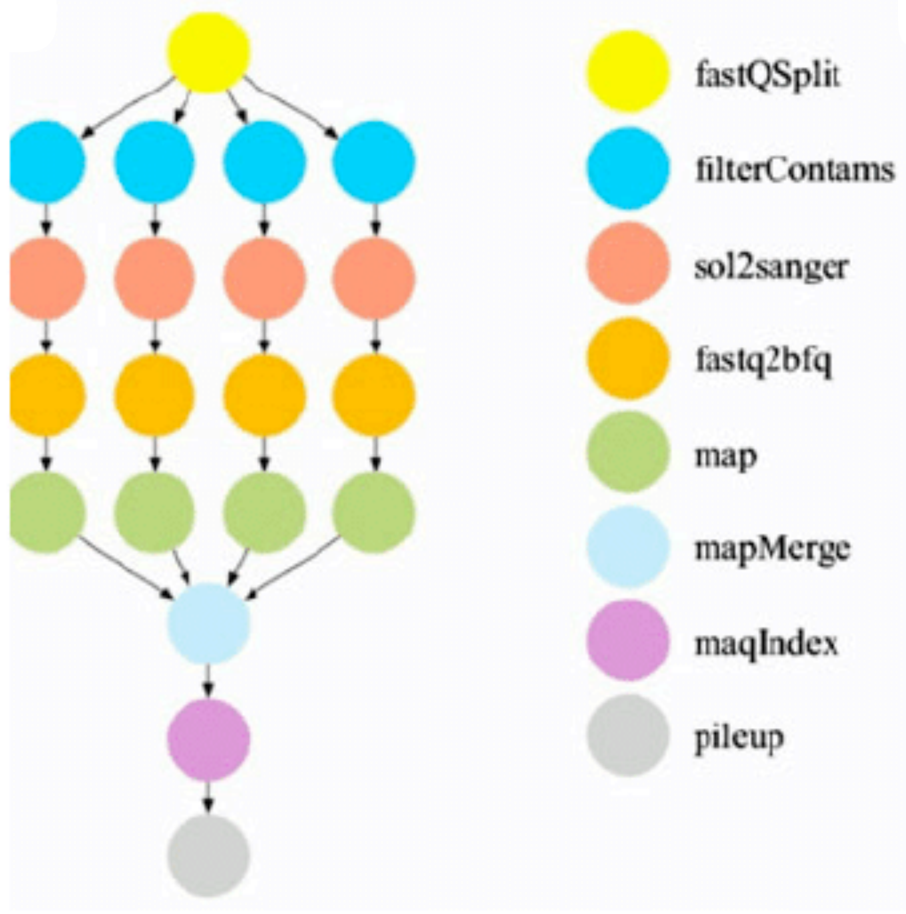
Bioinformatics

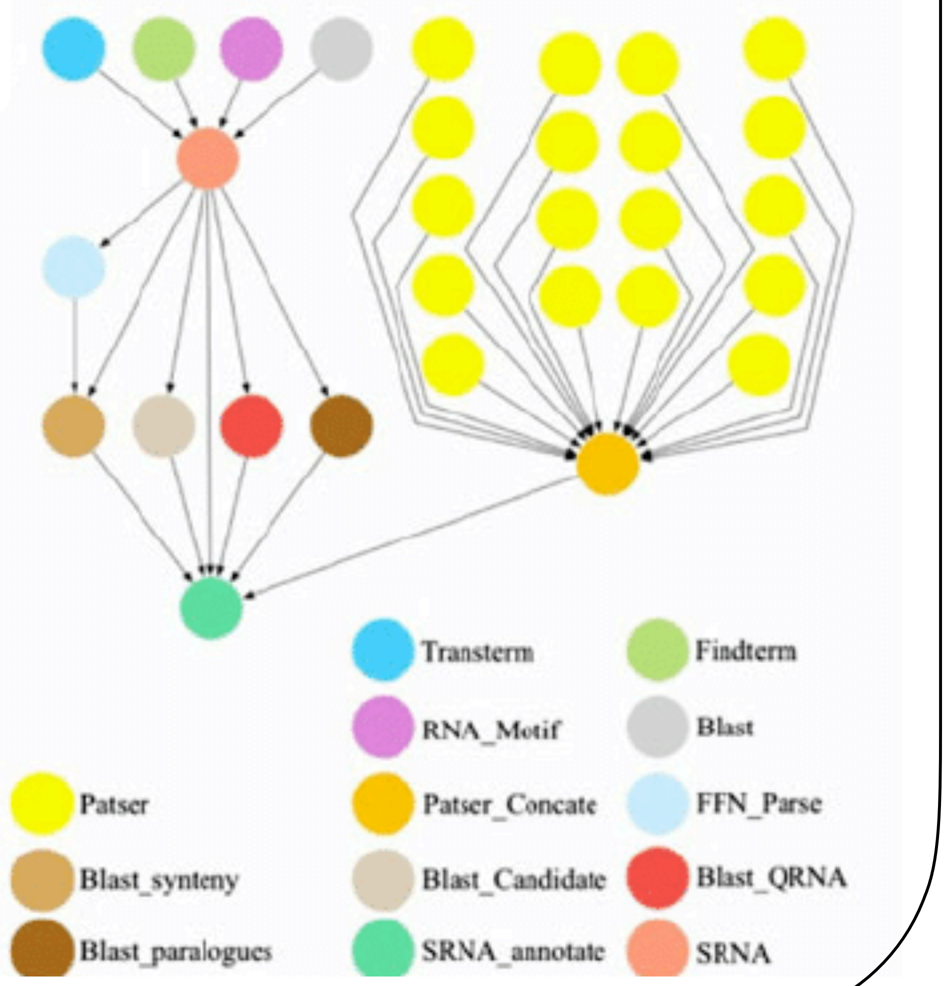
Seismology





Epigenomics





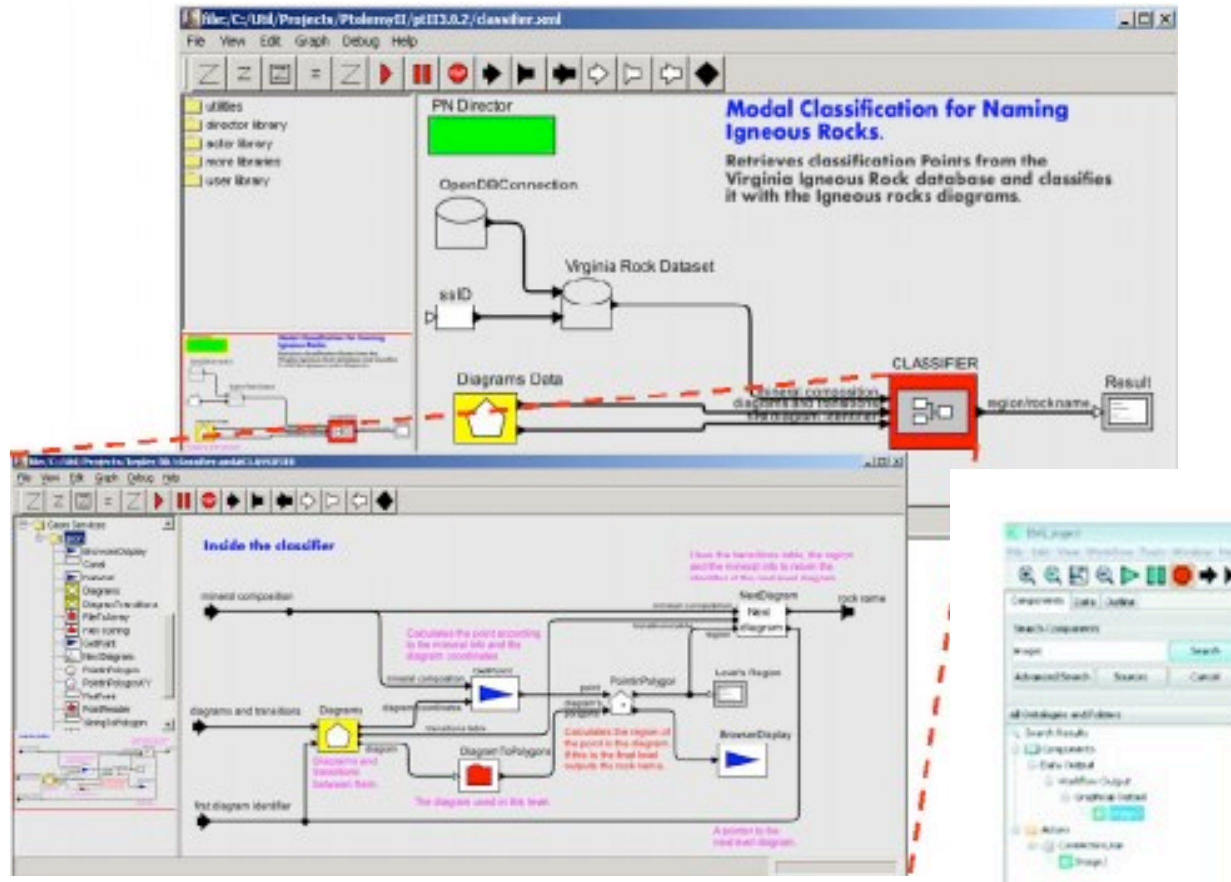
Apache Taverna

WorkflowHub

https://workflowhub.eu/workflows

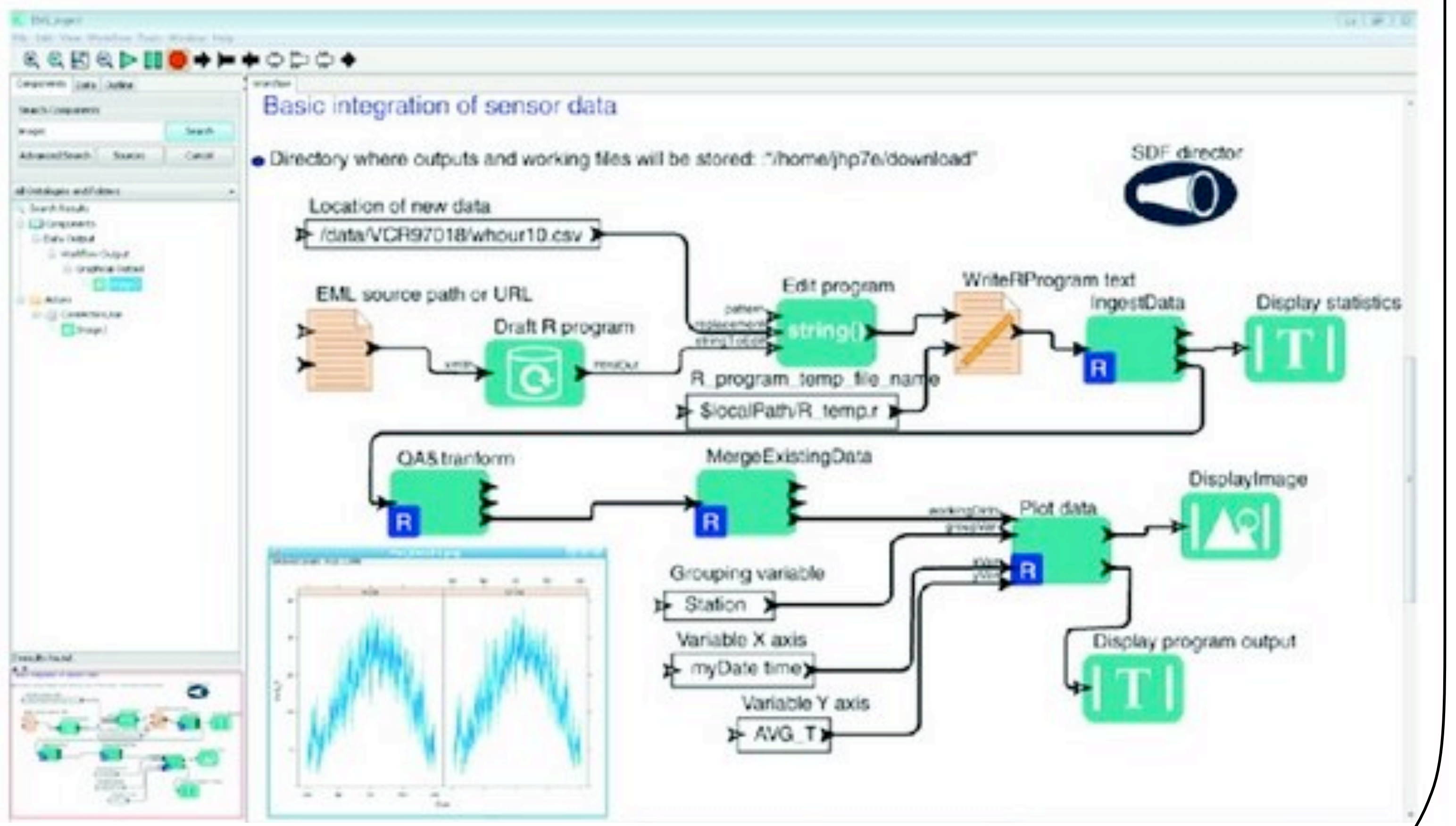
ASKALON

Geoscience



Kepler

Oceanography

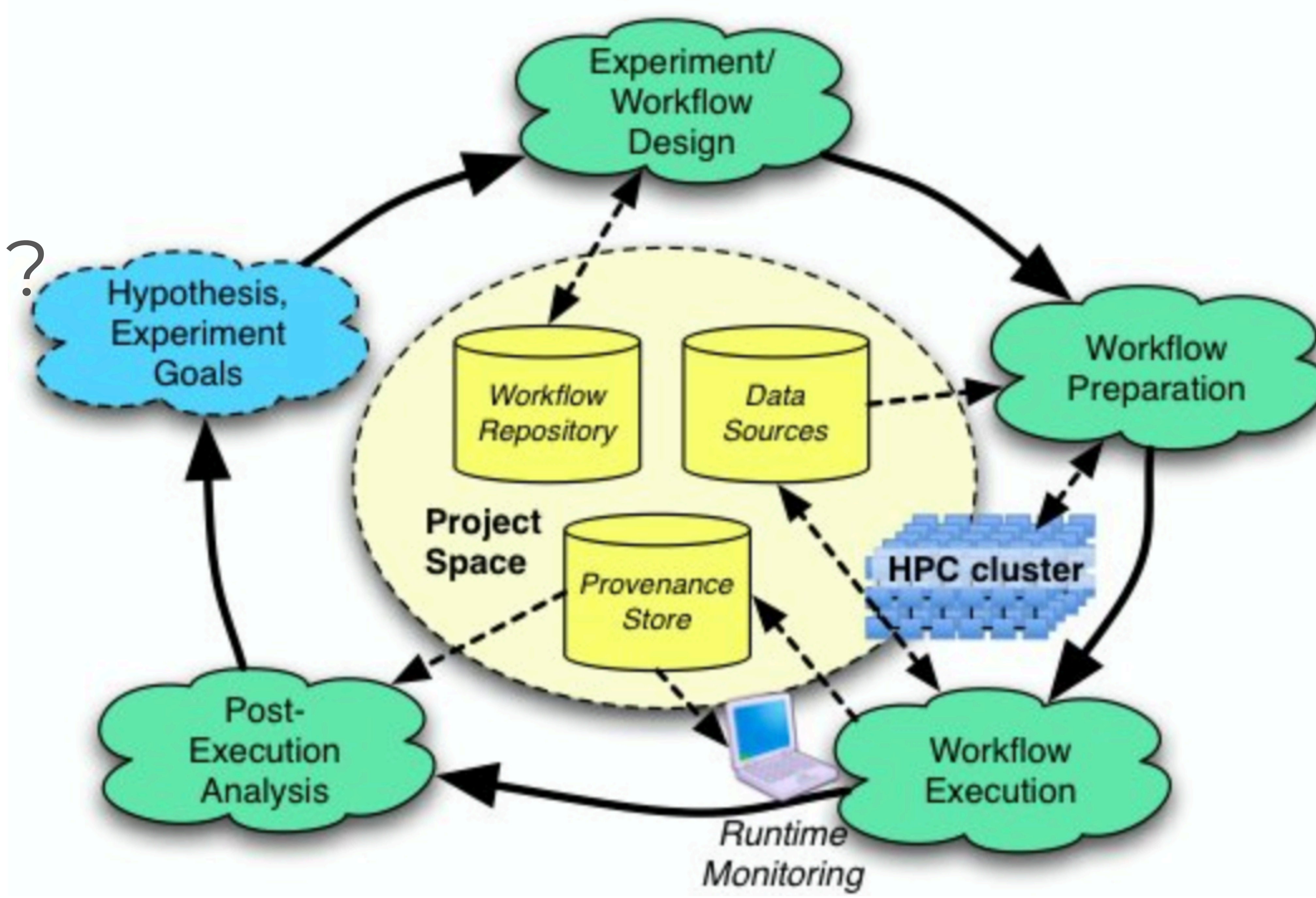


Source: https://pegasus.isi.edu/workflow_gallery/gallery/galactic/index.php

Souce: https://kepler-project.org/users/projects-using-kepler.html

Analytical Workflow Lifecycle

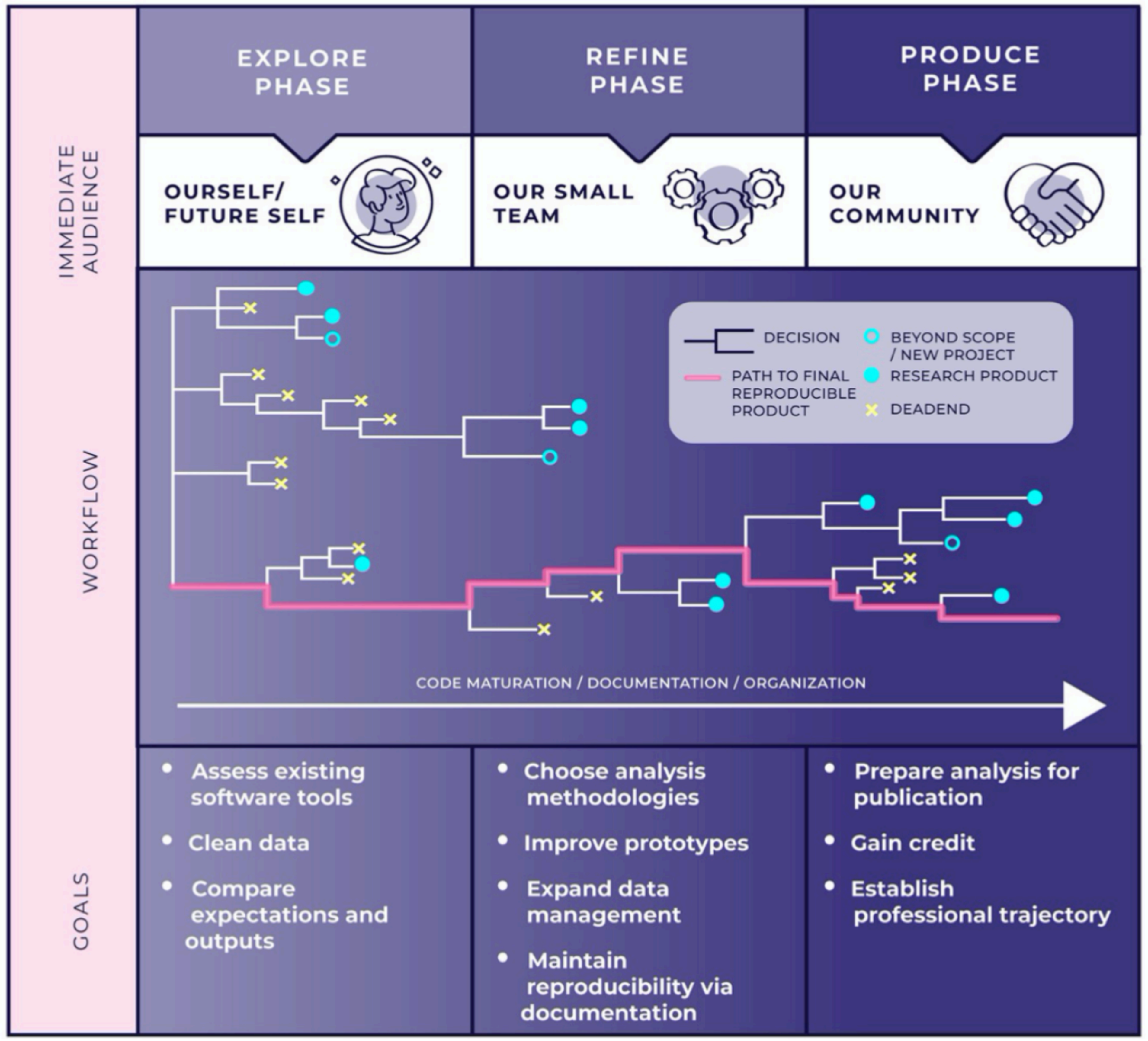
- What are the analytical steps you are anticipating?
- What are the dependencies among the various tasks?
- What is the amount of data needed?
- What computing power do you need?
- How will you share and preserve your work?
- Who is going to do what?

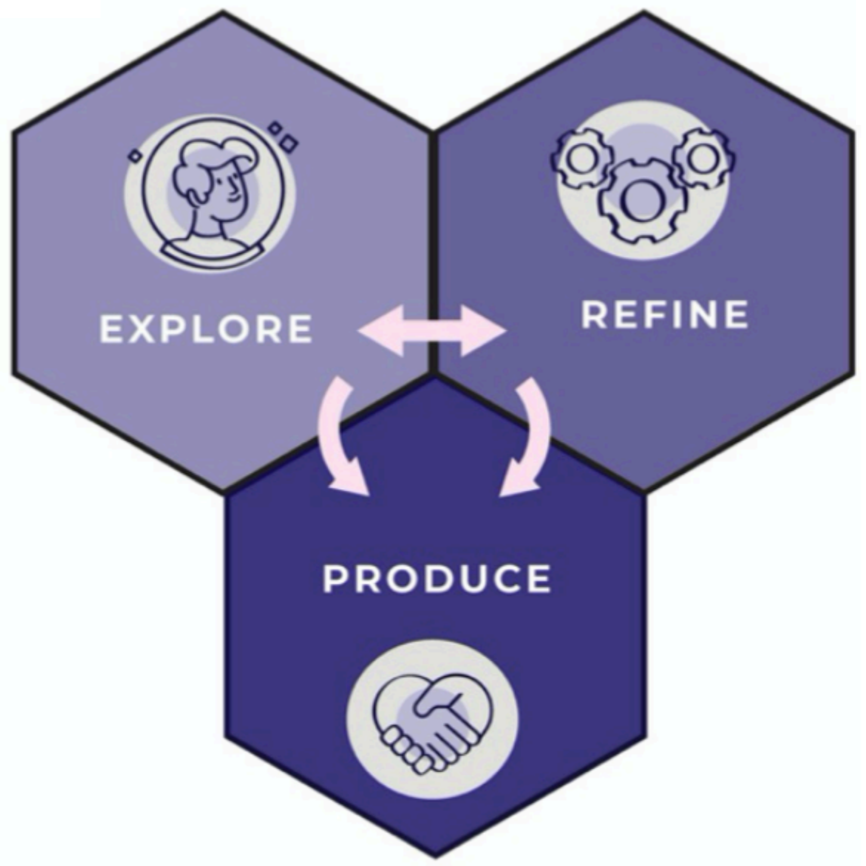


Data preparation is very time consuming (60-80% of a project)

Computational Reproducibility Concerns

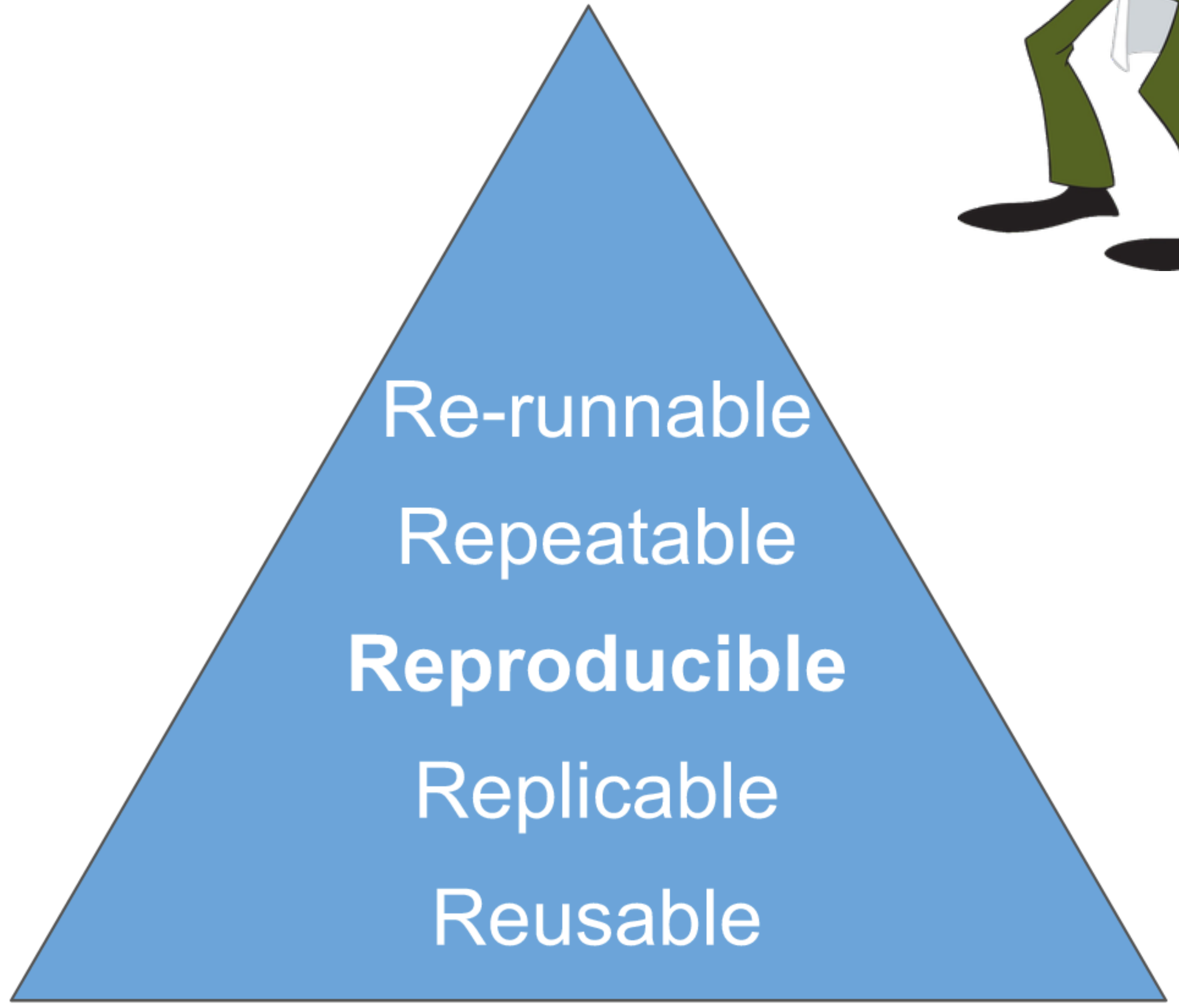
Reproducible research is the ability to recreate results given the same data, analytic code, and documentation.





Stoudt, S., Vásquez, V.N., Martinez, C.C., 2021. Principles for data analysis workflows. PLOS Computational Biology 17, e1008770. https://doi.org/10.1371/journal.pcbi.1008770

one-time use of your workflow



Contribution to your community

Outline

I. **Scientific Workflows and Analytical Workflows**
- Definitions and Differences
- Illustrative Examples

II. **Optimization in Analytical Workflows**
- Current Approaches
- Main Challenges

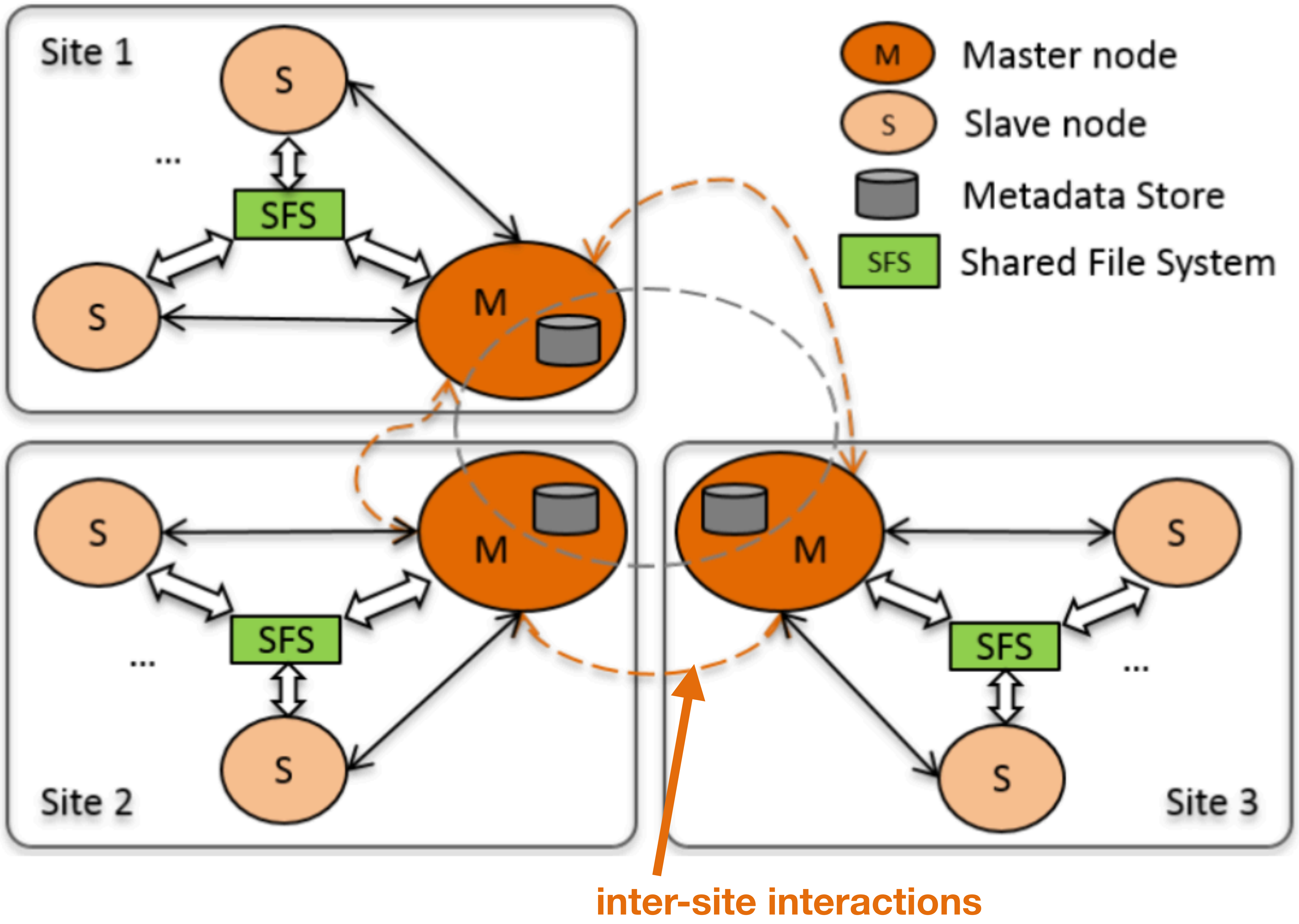
Architecture of Scientific Workflow Management Systems (SWMSs)

(Liu et al. , 2015)

Analytical Workflow Execution Plan

Multisite Workflow Execution Architecture

(Liu et al. , 2018)

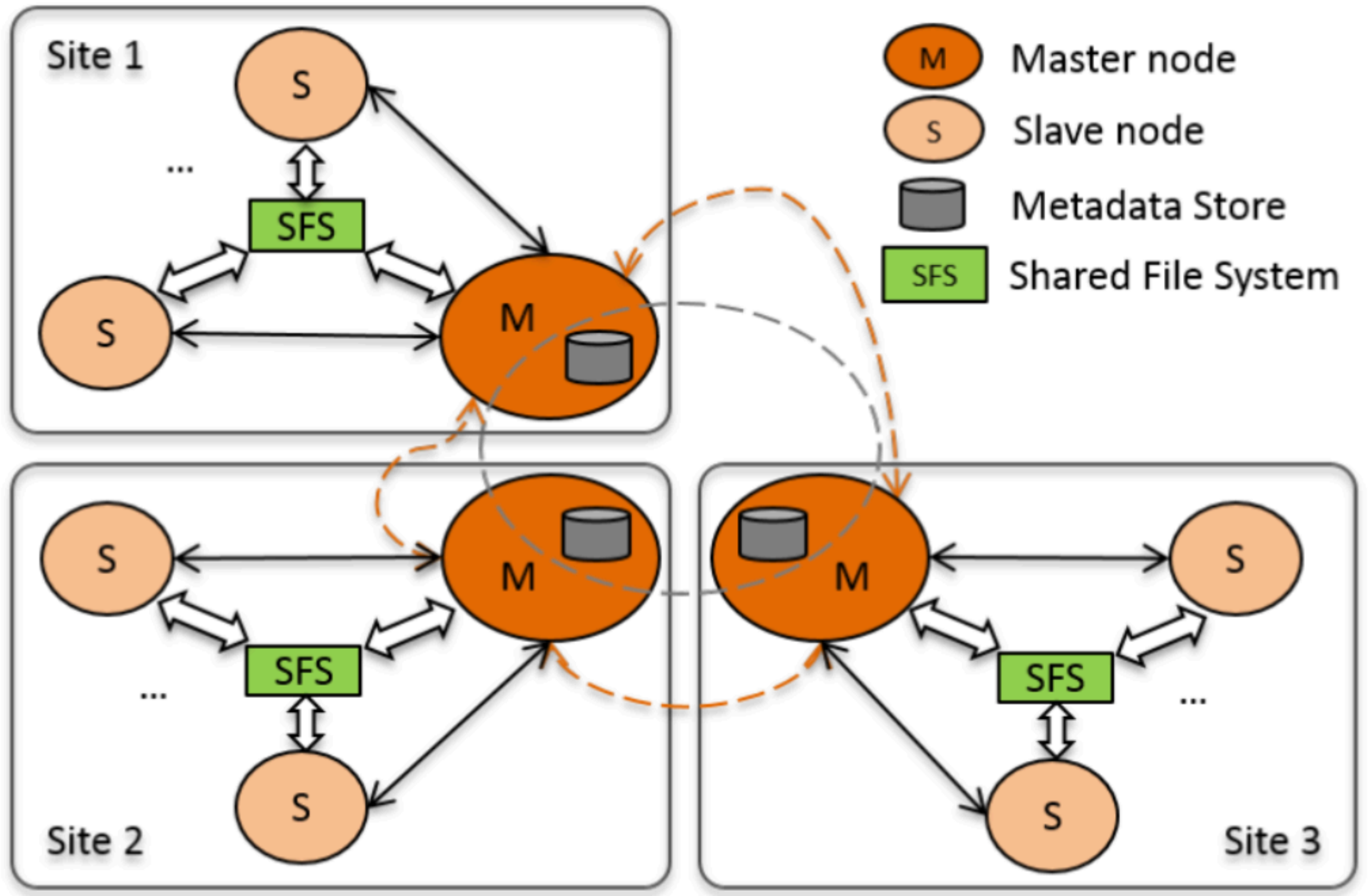


NoSQL databases: MongoDB, Cassandra

Examples of shared-disk file systems:
- General Parallel File System (GPFS),
- Global File System (GFS) and
- Network File System (NFS)

e.g., Amazon or Microsoft have many geographically distributed sites

Optimization in Analytical Workflows



Optimization Metrics

- Data transfer time/cost
- Computation time/cost
- Makespan and reliability
- Energy consumption (Warade et al., 2023)
- Users constraints
- QoS
- ...

Efficient Scheduling

- Finding a schedule for any DAG of tasks is an NP-hard
- Inefficiencies of current batch scheduling systems (Lubrano et al., 2024)
- Hardware can fail (fault-tolerance)
- Must consider task dependencies and resource requirements dynamically, DAG vs DCG
- Cloudlet scheduling is NP-complete (Ala'anzy et al., 2023) (Ghafir et al., 2023)
- Static/dynamic/hybrid scheduling

Handling massive data

- Different I/O performance metrics
- Complex data sharing and coordination (Hewes et al., 2023)
- Complex data provenance management
- Adaptive caching, hot and cold data in main-memory, cache service (Qin et al., 2019)
- Metadata management bottleneck

Efficient Scheduling

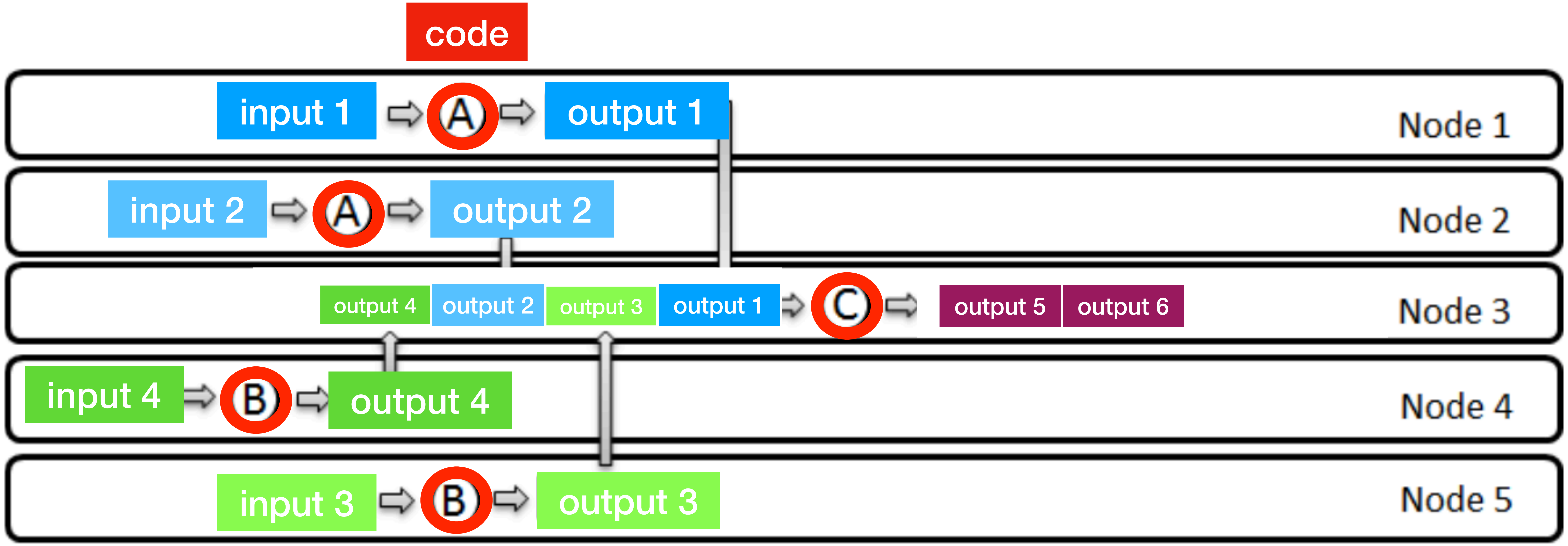
Fine-grained Parallelism in SWMSs

data parallelism

pipeline parallelism

independent parallelism

Hybrid parallelism



(Liu et al. , 2015)

Efficient Scheduling

Workflow Scheduling

Mapping the workflow tasks generated by workflow parallelization to the physical resources

- Architecture
  - Monosite
  - Multisite
- Mode
  - Static
  - Dynamic
  - Hybrid
- Method
  - Heuristics
  - Meta-heuristics
- Objective
  - Single
  - Multiple
    - Execution time
    - Data transfer time/cost
    - Compute cost
    - Usage charge period
    - VM per task
    - VM cores
    - VM overhead cost/time

Efficient Scheduling

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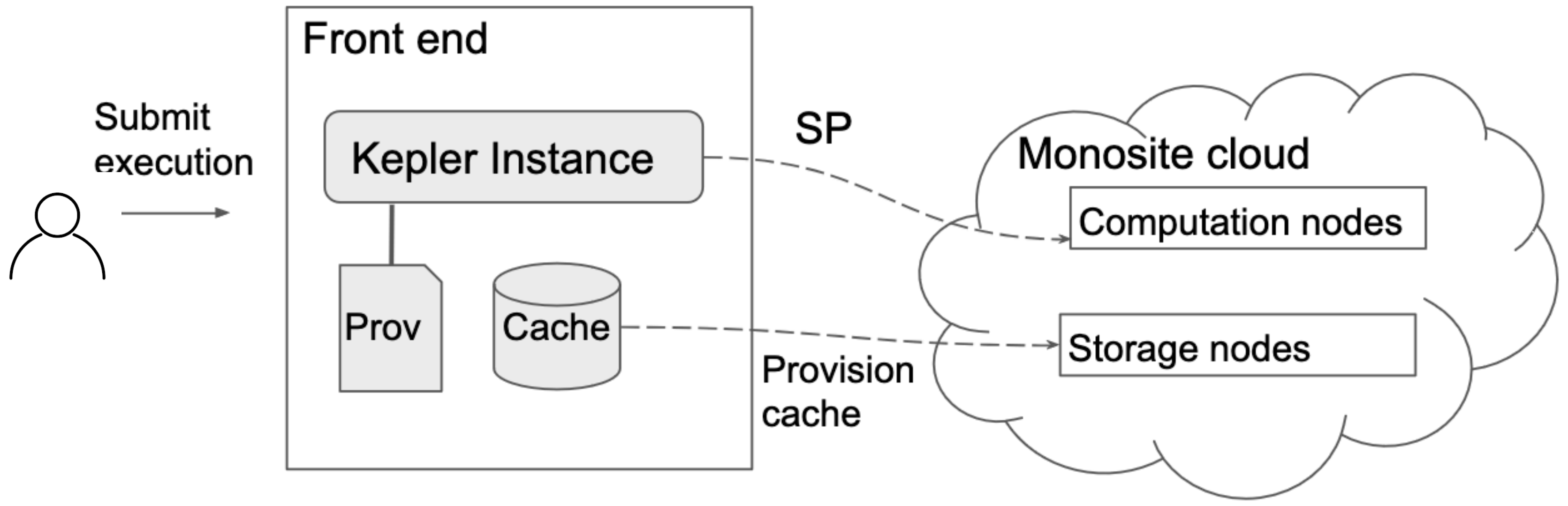
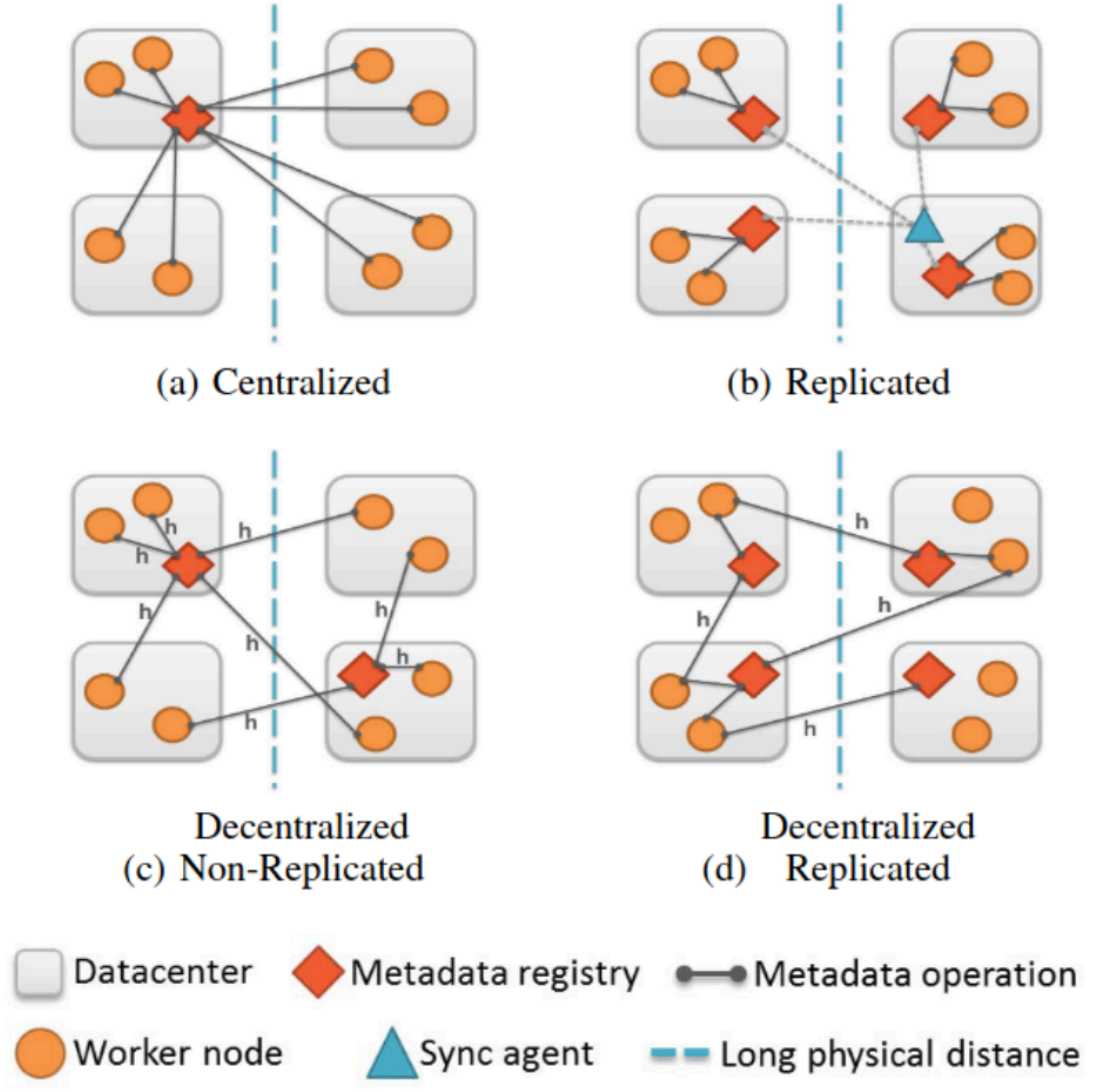
Kepler



Handling massive data

Management Strategies for Distributed Workflow Metadata

(Pineda-Morales L. et al., 2018)

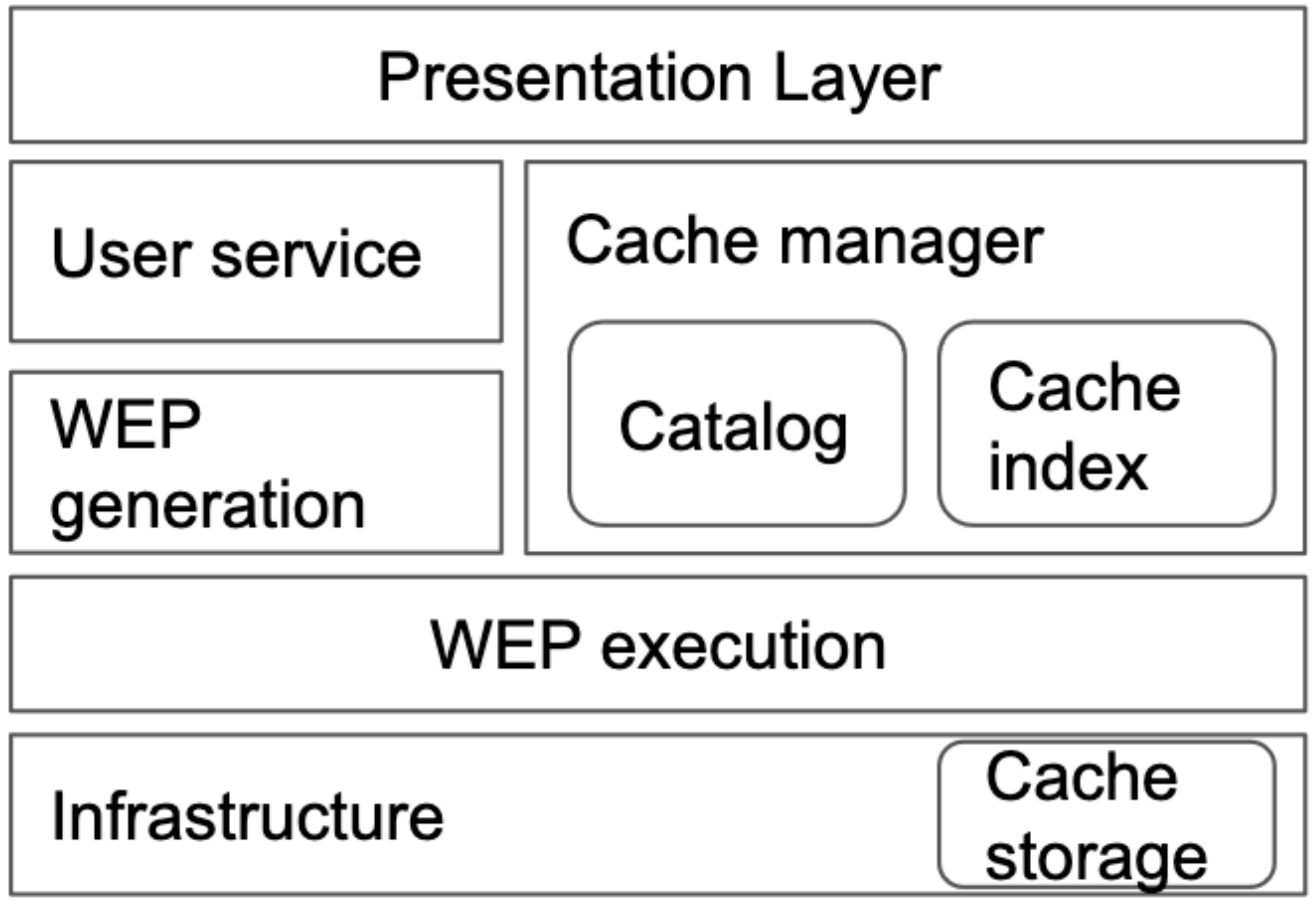


Handling massive data

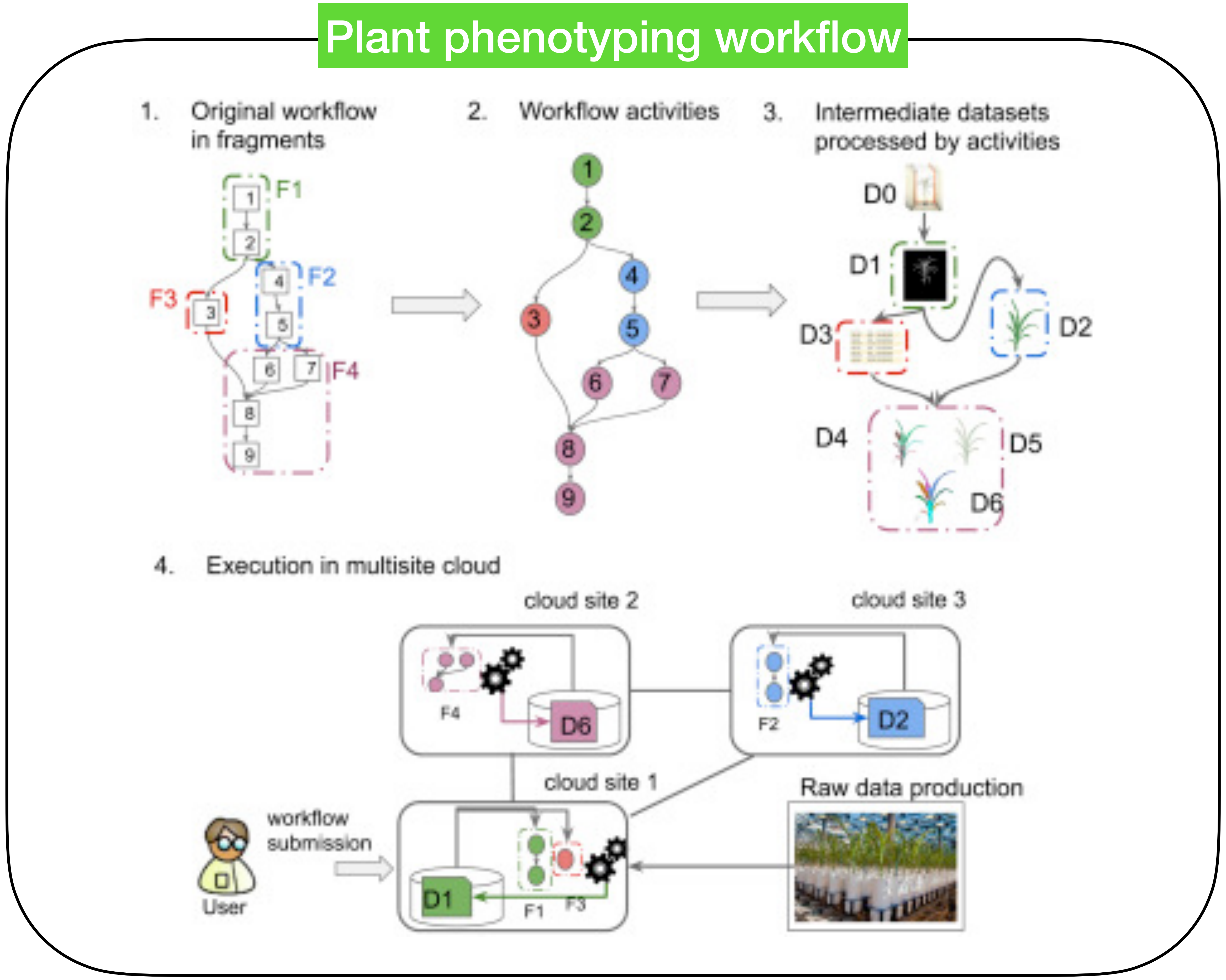
Data Caching

1) Which intermediate data should be shared, stored, or replicated? **Where**? **When**?

2) Which existing cached data should be reused?



Generic Architecture of SWMS with Cache Management



Cache-Aware scheduling (Heidsieck, et al. 2021)

Concluding Remarks

- Scientific workflows become increasingly complex with simulation data, large-scale experiment data, synthetic data, GenAI data, etc.
- Orchestration between the workflow tasks, the distributed computing and data storage resources is challenging and requires various expertises and R&D in data management, HPC, and optimization.
- Metadata management is a keystone for optimizing scientific workflows.
- Still research is needed for optimizing the next generation of scientific workflows involving deep learning, pre-trained models, LLMs, and multimodal GenAI data.

Thanks!

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https://laureberti.github.io/website/

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