Exploring Scientific Workflows with CWL and dispel4py

Module 1.a

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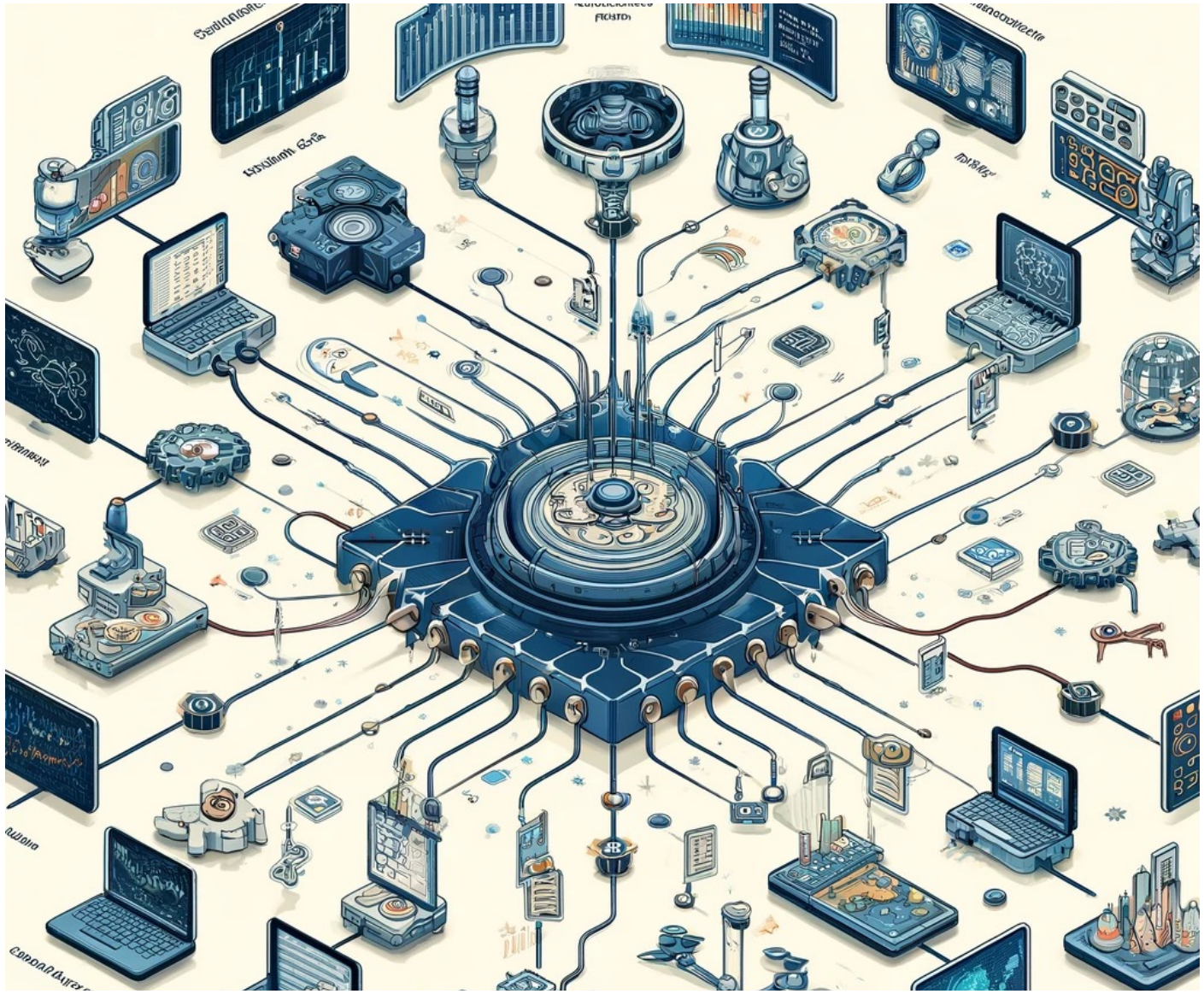
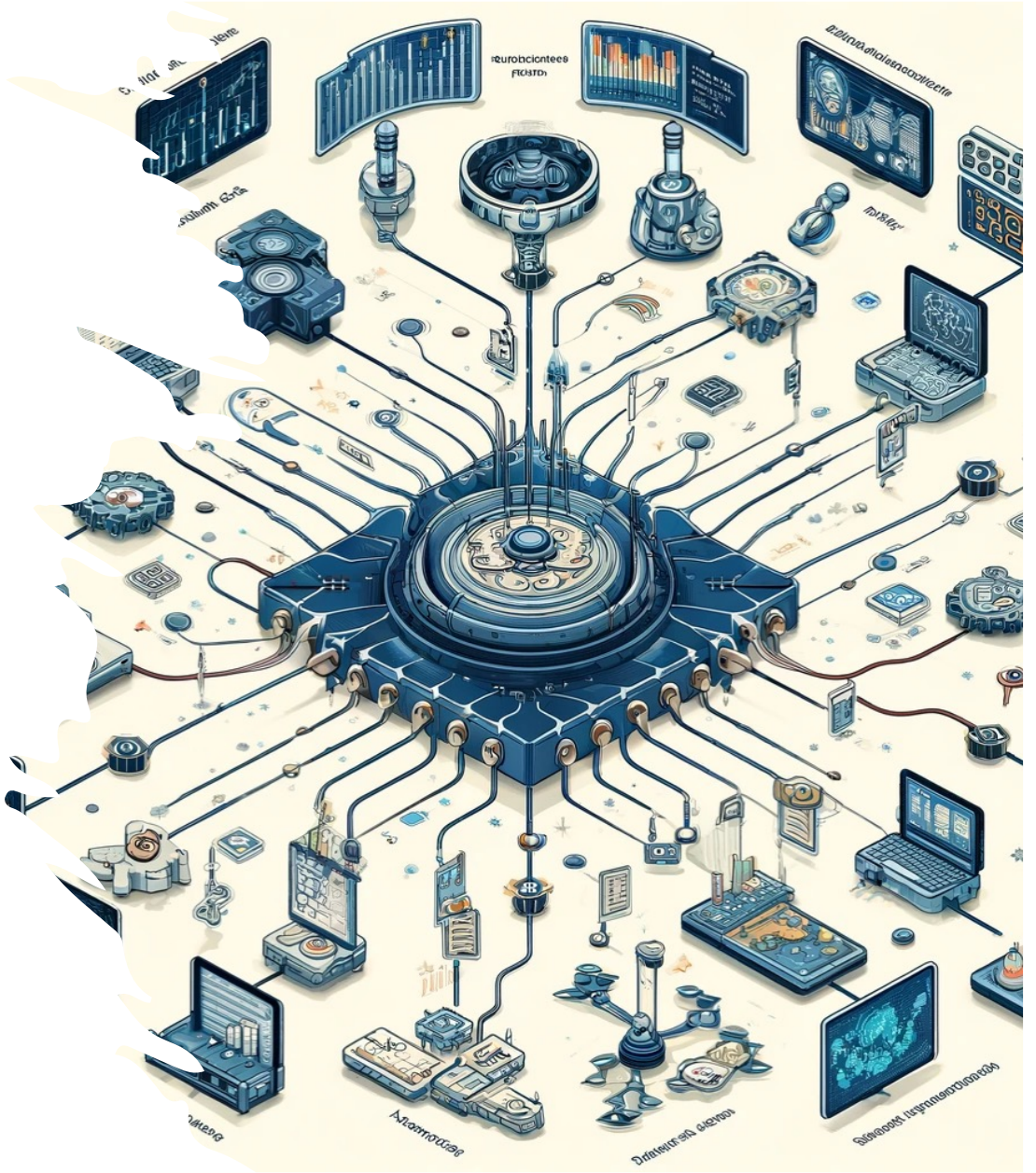


Seminar Overview

- Day 1: Understanding Scientific Workflows (4 Hours)
  - Module 1: Introduction to Scientific Workflows
    - Module 1.a
      - Defining scientific workflows and WMS
      - How to Select WMS
    - Module 1.b
      - Beyond the Basics Concepts
      - Research Directions
  - Module 2: Creating Workflows with CWL
- Day 2: Exploring dispel4py and its applications (4 Hours)
  - Module 3: Introduction to dispel4py
  - Module 4: Comparative Analysis and Real-World



Module 1.a- Introduction to Scientific Workflows

1. Defining scientific workflows and Workflows Management Systems (WMS)
   i. Workflow Definition and Importance
   ii. Historical Context
   iii. You might use workflows already
   iv. Workflow Key Phases
   v. Workflow High-Level Elements
   vi. Workflow Management Systems (WMS)
2. How to Select WMS
   i. Key Factors to Consider
   ii. Interface
   iii. Workload
   iv. Community
   v. Task-Flow vs Data-Flow
   vi. Real Examples

1. Defining scientific workflows & Workflow Management Systems (WMS)

Workflow Definition and Importance

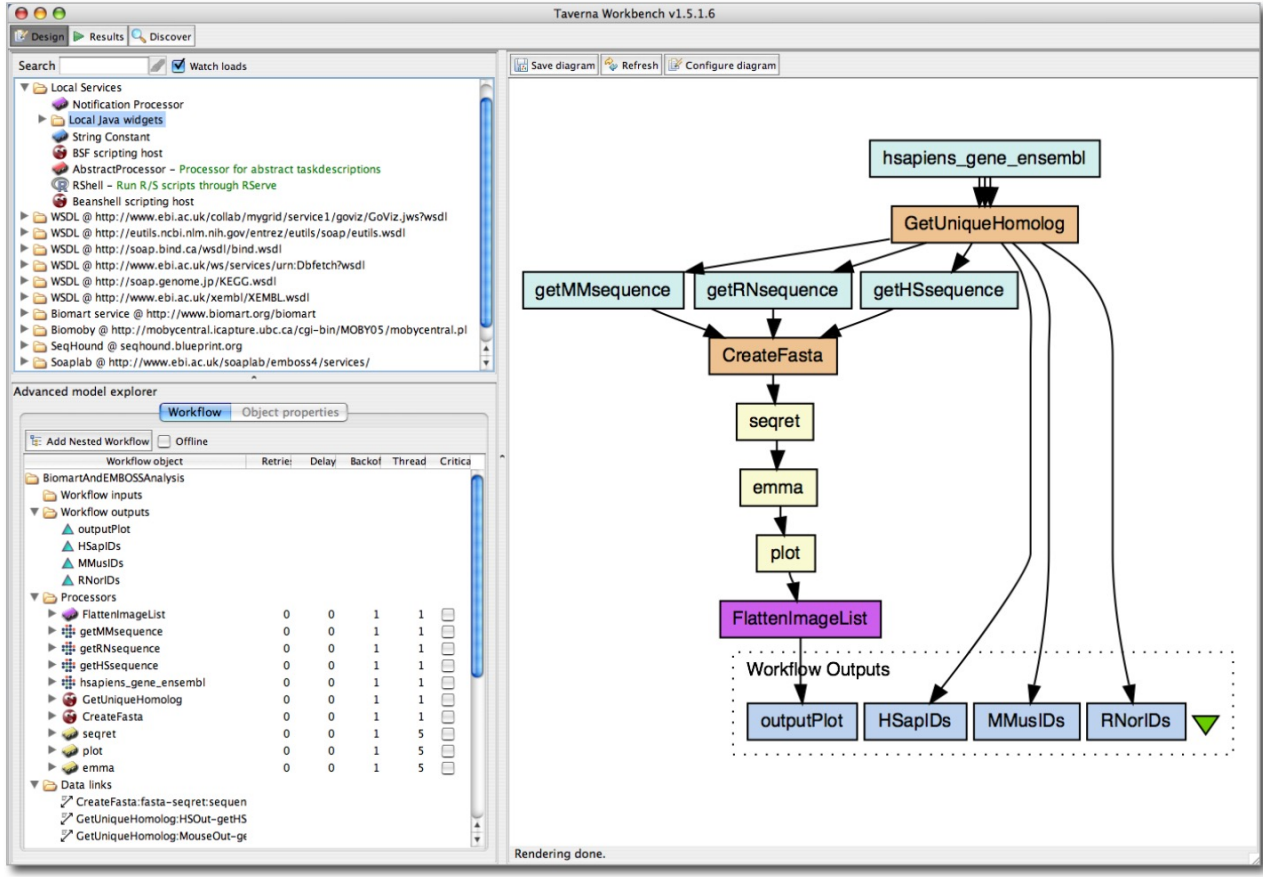
- Workflows refer to the structured sequences of:
  - Data processing
  - Analysis tasks
- Workflows are crucial for ensuring:
  - Systematically execution of complex and multi-step processes/tasks
    - Facilitate the organization of tasks
  - Verifiable and reproducible results.
    - Enhance the efficiency and reliability of scientific research.

Workflow Definition and Importance

- Formal way to express a calculation
- Multiple tasks with dependencies between them
- No limitations on tasks
  - Short or long
  - Loosely or tightly coupled
- Capture task parameters, input, output
- Independence of workflow process and data
- Often, run same workflow with different data

Workflow Definition and Importance

- Example workflow represented in the Taverna workflow system.
  - Extracts gene IDs from human chromosome 22 with mappings to disease functions and homologues in mouse and rat
  - Fetches base pairs of the associated DNA sequences;
  - Combines the sequences into a FASTA file;
  - Performs a multiple sequence alignment;
    - soaplab-based operations (seqret, emma, plot)
  - Renders the results



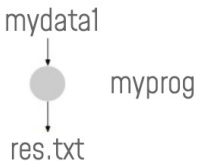
Historical Context

- The concept of workflows in science has evolved
  - from manual paper-based processes → highly automated systems
- This evolution has been driven by
  - increasing complexity of scientific research
  - processing & analysing large volumes of data.
- Scientific workflows are integral to a wide range of disciplines:
  - BioInformatics
  - Astronomy
  - NeuroInformatics
  - GeoSciences
  - Social Sciences ….

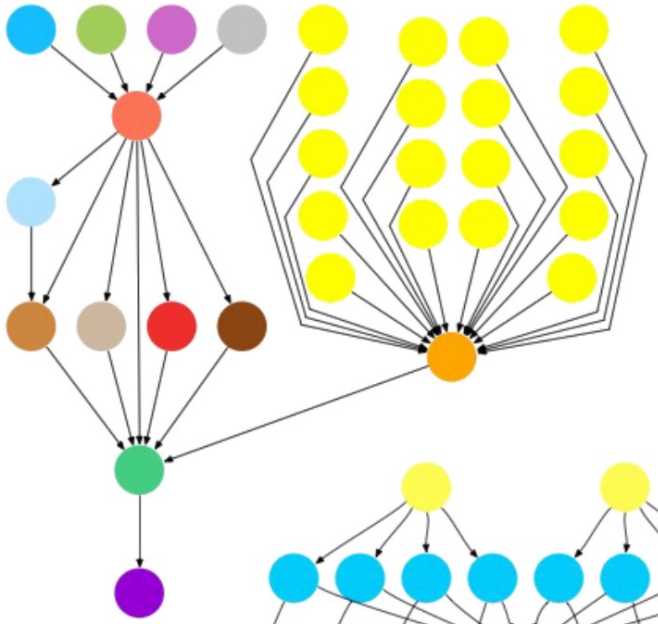
Historical Context

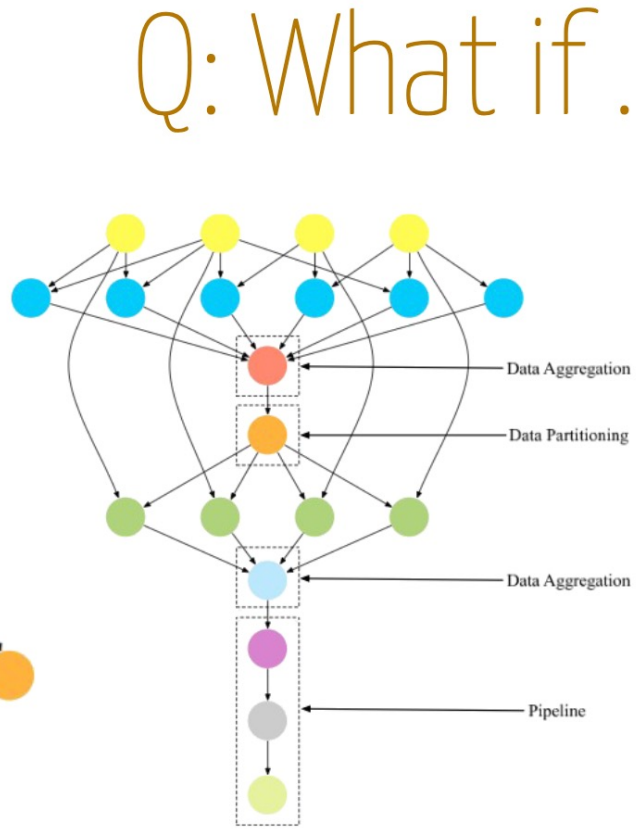
- What do you do when to want to run computations on a cluster ?
  - you write a submission script and submit it to the scheduler (e.g. Slurm) ?

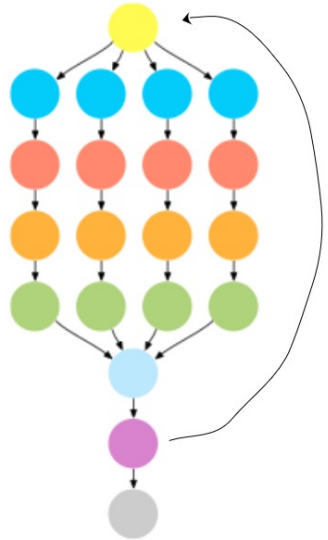
```
#!/bin/bash
# Submission script for demonstrating
# slurm usage.

# Job parameters
#SBATCH --job-name=demo
#SBATCH --output=res.txt
# Needed resources
#SBATCH --ntasks=1
#SBATCH --mem-per-cpu=2000
#SBATCH --time=1:00:00

# Operations
echo "Job start at $(date)"
# Job steps
srun ~/bin/myprog < mydata1

echo "Job end at $(date)"

~
                              19,0-1        All
```



Historical Context







You need workflows !

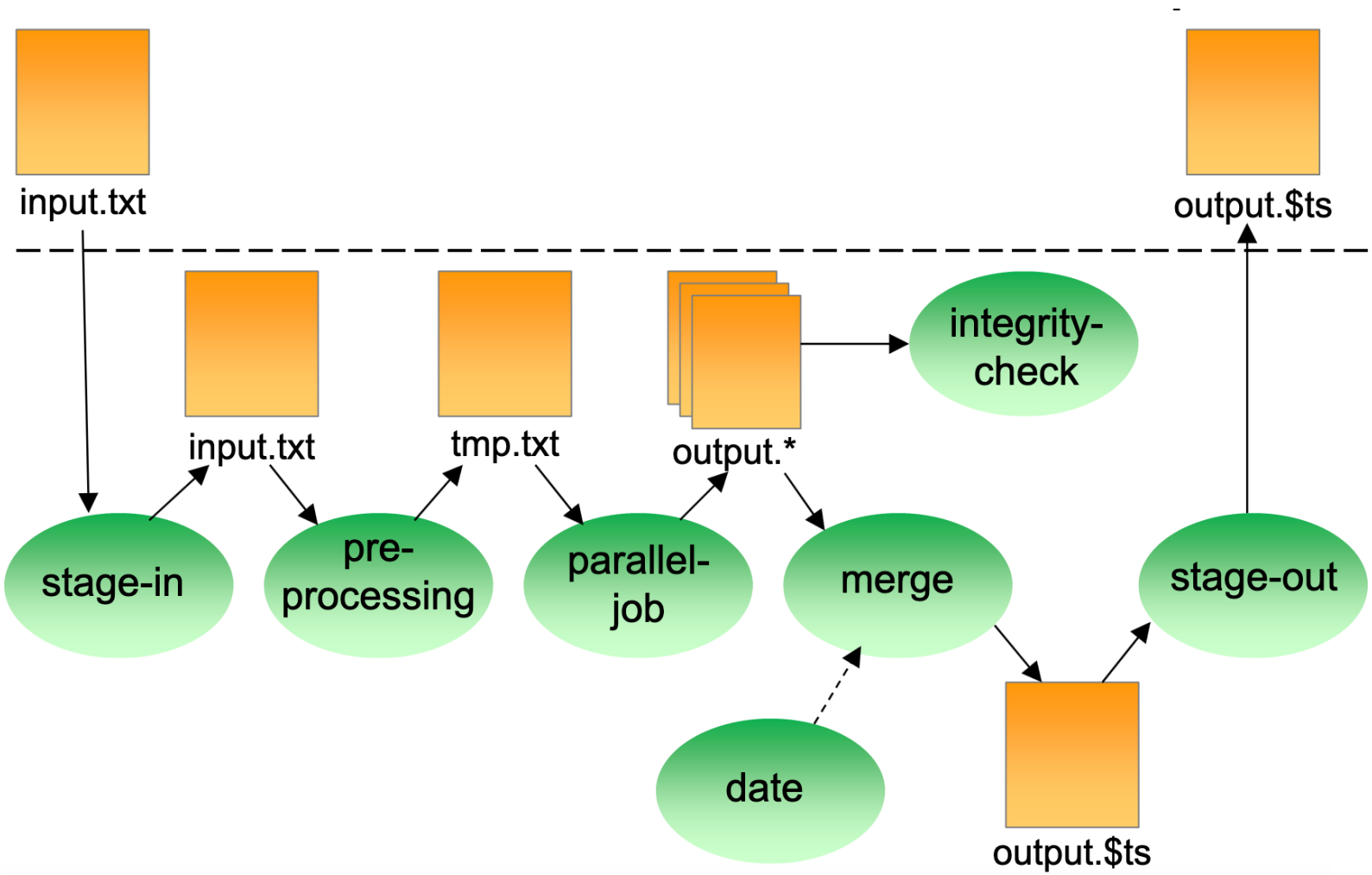
You might use workflows already

Example of a Shell Script "*Workflow*"

```
#!/bin/bash
1) Stage-in input data to compute environment
scp myself@datastore.com:/data/input.txt /scratch/input.txt
2) Run a serial job with an input and output
bin/pre-processing in=input.txt out=tmp.txt
3) Run a parallel job with the resulting data
mpiexec bin/parallel-job in=tmp.txt out_prefix=output
4) Run a set of independent serial jobs in parallel – scheduling by hand
for i in `seq 0 $np`; do
      bin/integrity-check output.$i &
done
5) While those are running, get metadata and run another serial job
ts=`date +%s`
bin/merge prefix=output out=output.$ts
6) Finally, stage results back to permanent storage
scp /scratch/output.$ts myself@datastore.com:/data/output.$ts
```

You might use workflows already

Schematic of the Shell Script "*Workflow*"



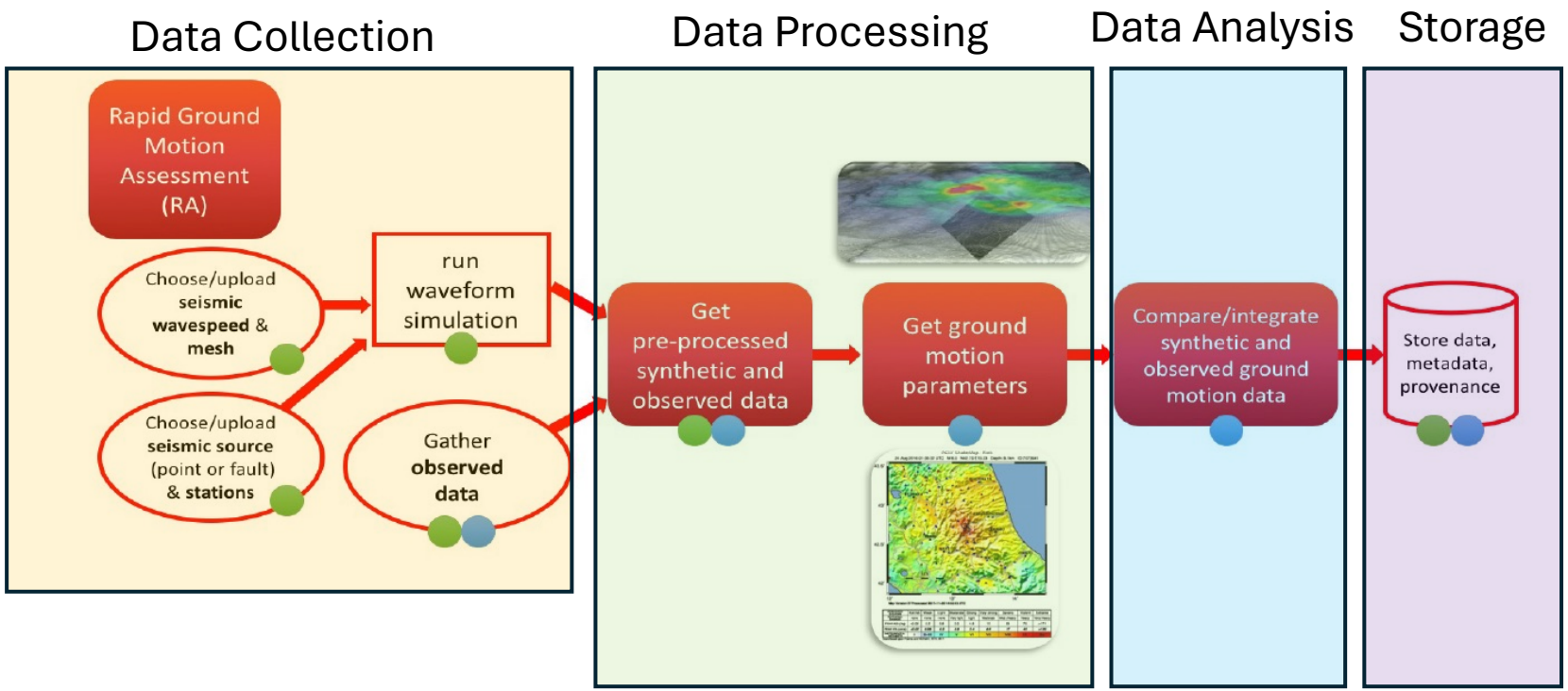
Workflows Key Phases

- Data Collection
  - acquiring raw data from experiments or simulations
- Data Processing
  - cleaning and structuring data for analysis
- Data Analysis
  - applying statistical models and algorithms to interpret data
- Visualization & Storage
  - creating graphical representations of analysis results
  - storing the results/metadata/provenance for further analysis

These components are interconnected in a workflow. Lets see an example!

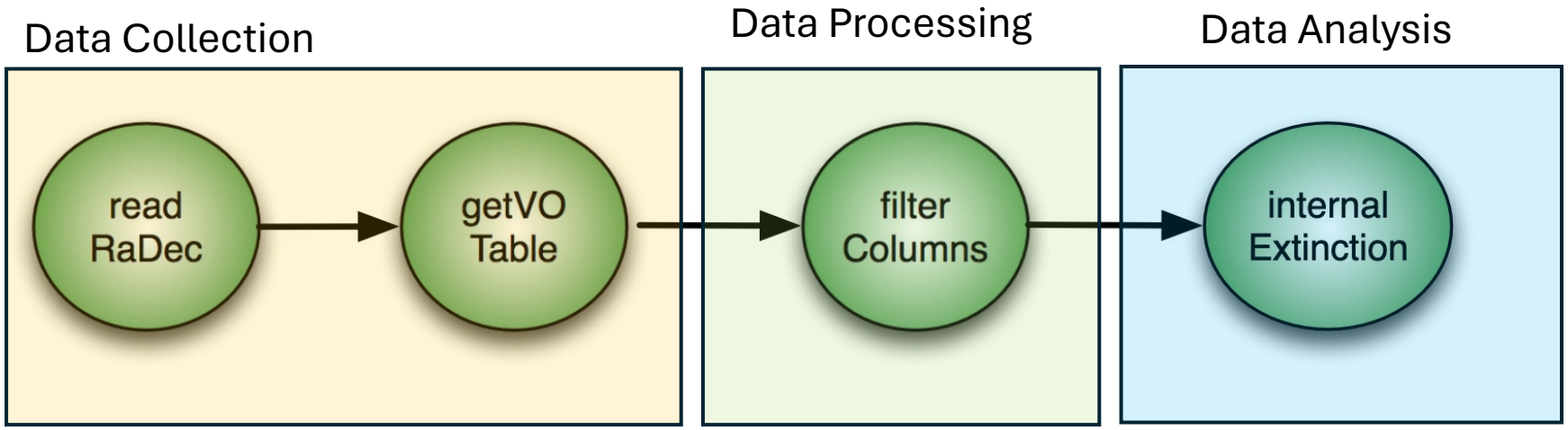
Workflows Key Phases

- Seismological Example:
  - Quickly analyze earthquakes
  - Model the ground motion after earthquakes
  - Rapid assessment of earthquakes' impact, and emergency response



Workflows Key Phases

- Astrophysics:
  - Calculating the Internal Extinction of Galaxies from the AMIGA catalogue
  - Crucial for determining a galaxy's optical luminosity.



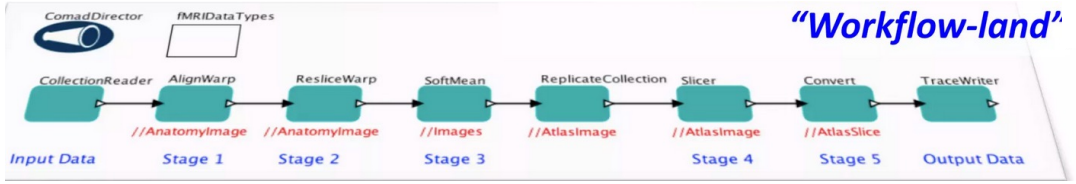
Workflow High-level Elements

- Task executions with dependencies
  - Specify a series of tasks to run
    - Data Collections, Data pre-processing and simulation
    - Data Analysis, Visualization, Storage
  - Outputs from one task may be inputs for another
    - DataFlow management – using streams/data between tasks
    - File management - using files between tasks
- Task scheduling
  - Some tasks may be able to run in parallel with other tasks
- Resource provisioning (getting processors)
  - Computational resources are needed to run jobs
- Ensuring accuracy and efficiency
  - Provenance generation – what is provenance in workflows ?

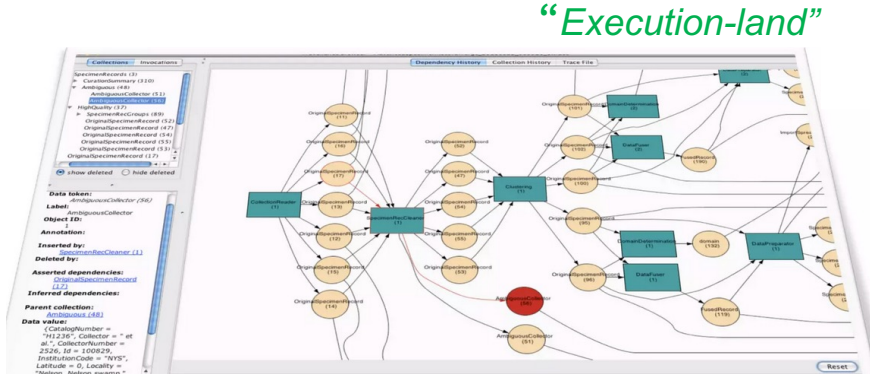
Workflow High-Level Elements

- Provenance:
  - Capturing information about the workflow
    - E.g. when a task was run ?; with which parameters?; what was the previous task ? And the next one ? ….
  - Enables reproducibility of results, transparency, data sharing
- Two types:
  - Prospective provenance
  - Retrospective provenance

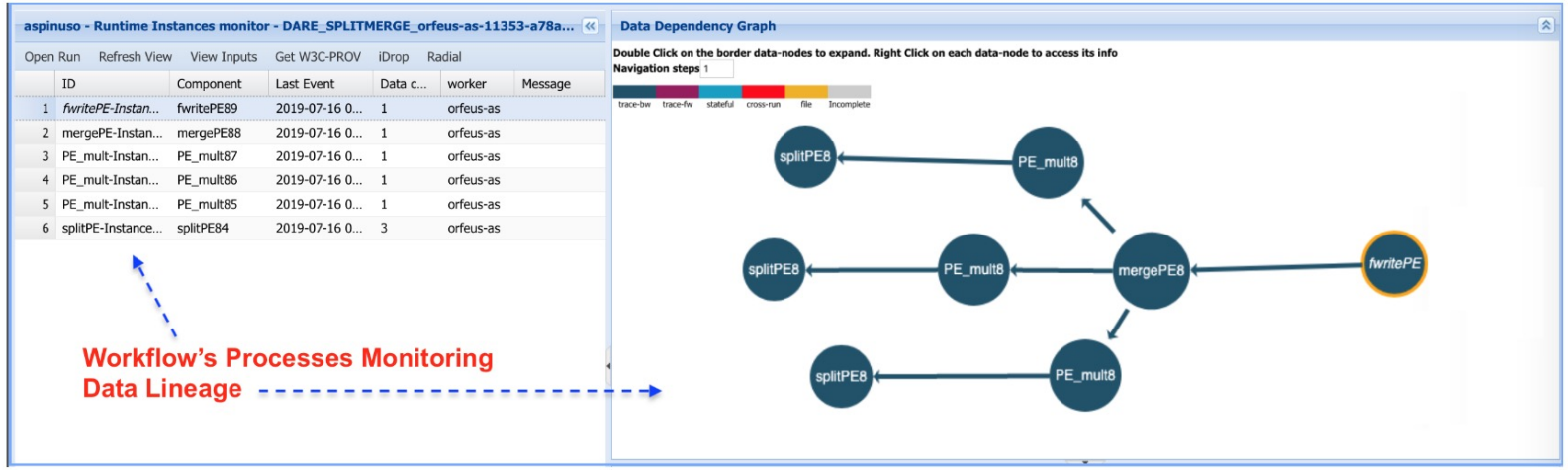
- Prospective provenance:
  - captures the **structure and static context** of a workflow
  - it is independent of workflow execution or input data
  - provides an **abstract overview** of a workflow



- Retrospective provenance (~ tracing/profiling in HPC) :
  - captures the **information about a workflow's execution**
  - becomes available when **running the workflow**.
  - facts about the execution of each workflow step & runtime environment



Workflow High-Level Elements



dispel4py provenance visualization of the execution of the Split and Merge workflow

retrospective provenance →includes facts about the execution of each workflow step and the runtime environment

What do we need help with?

- Task executions with dependencies
  - What if something fails in the middle?
  - Dependencies may be complex
- Task scheduling
  - Minimize execution time while preserving dependencies
  - May have many tasks to run
- Resource provisioning
  - May want to run across multiple systems
  - How to match processors to work?

What do we need help with?

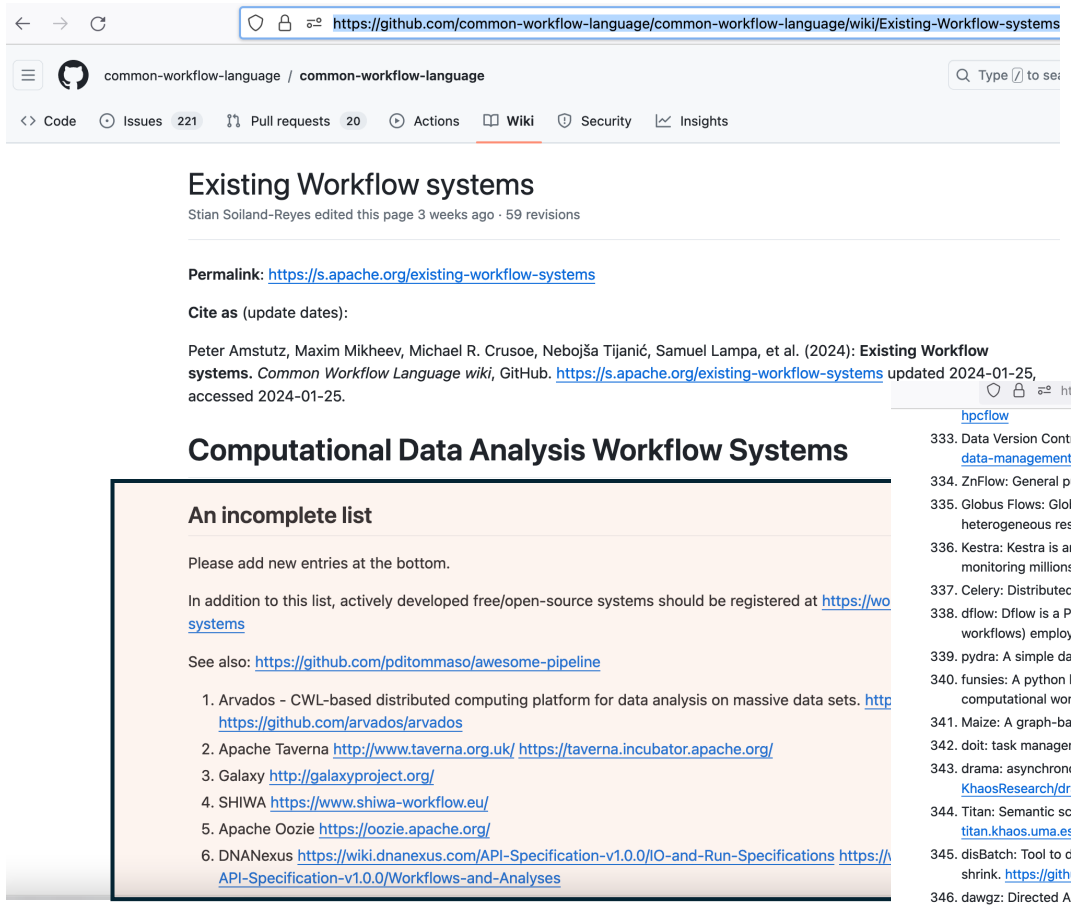
- Metadata and provenance
  - Automatically capture and track
  - Where did my task run? How long did it take?
  - What were the inputs and parameters?
  - What versions of code were used?
- File & Data management
  - Make sure inputs are available for tasks
  - Archive output data
- Automation
  - You have a workflow already – are there manual steps?

Workflow Management Systems (WMS)

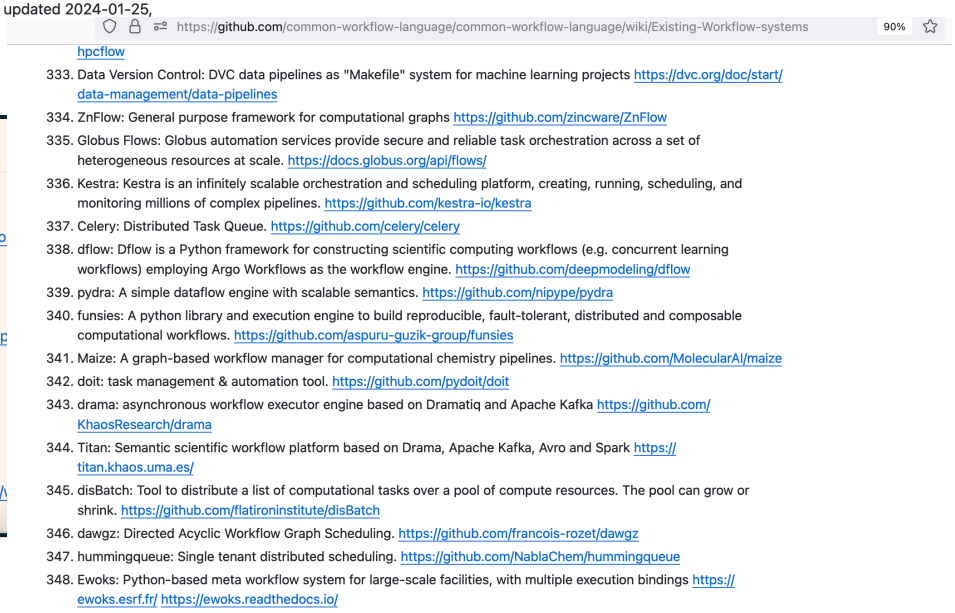
- Workflow Management Systems (WMS)
  - Software solutions that provide the infrastructure for
    - Designing
    - Executing
    - Monitoring scientific workflows
  - They offer tools for
    - automating tasks
    - managing data flow
    - ensuring that computational resources are used efficiently

- Pegasus, Taverna, CWL, dispel4py, Apache Airflow, Nextflow, pycompss, ….
  - https://github.com/common-workflow-language/common-workflow-language/wiki/Existing-Workflow-systems
  - https://workflows.community/systems
  - Bringing the Scientific Workflows Community Together

Workflow Management Systems (WMS)



348 entries!

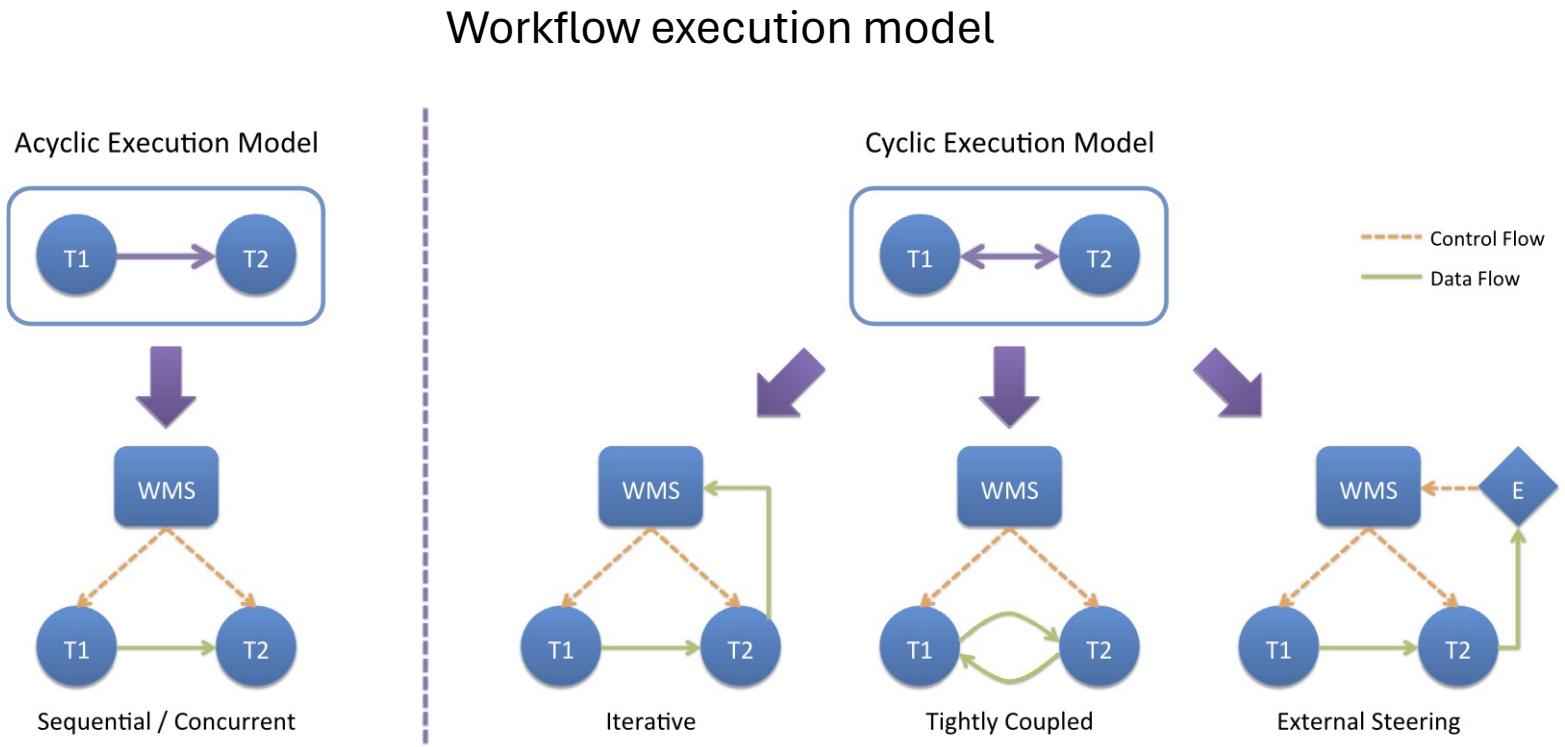


https://github.com/common-workflow-language/common-workflow-language/wiki/Existing-Workflow-systems

Workflow Management Systems (WMS)

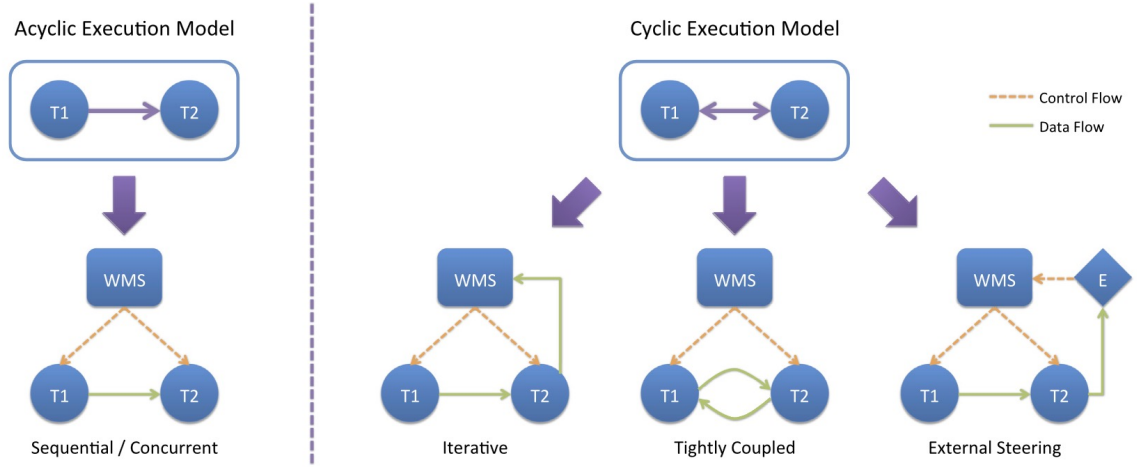
- Essential functions:
  - **Automate** programs and services scientists already use
  - **Support** one or several workflow execution modes.
  - **Schedule** invocation of programs and services correctly and efficiently – in **parallel** where possible.
  - **Manage dataflow** to, from and between programs and services
  - **Enable scientists (**no just developers) to author and modify workflow easily
- Desired functions:
  - **Predict** what a workflow will do when executed: **prospective provenance**.
  - **Record** wat happened during workflow execution: **retrospective provenance**
  - **Reveal and query provenance –** how workflow products were derided from inputs
  - Enable scientists to **version, share** and **publish** their workflows

Workflow Management Systems (WMS)



A characterization of workflow management systems for extreme-scale applications

Workflow Management Systems (WMS)



- **Sequential**:
  - Begins with T1 followed by T2 upon completion;
  - Ideal for processes involving a simulation followed by post-processing.
- **Concurrent**:
  - T1 and T2 run simultaneously . T1's output feeding into T2;
  - Suitable for streaming data and multiple-stage processing
- **Iterative**:
  - Repeating sequences where T1's completion leads to T2, and T2's results may trigger further iterations
  - Useful for exploring parameter spaces through Uncertainty Quantification (UQ).
- **Tightly Coupled**:
  - T1 and T2 exchange partial results;
  - Supporting closely integrated simulations (e.g. multi-physics simulations that require tight coordination)
- **External Steering**:
  - Similar to concurrent but includes user/system evaluation of T2's output to potentially adjust T1 or other workflow aspects;
  - Useful for scenarios requiring real-time analysis feedback to guide subsequent steps

1.vi) Workflow Management Systems (WMS)

Classification of workflow management systems

Workflow Properties	ADIOS	Airavata	Askalon	Bobolang	dispel4py	Fireworks	Galaxy	Kepler	Makeflow	Moteur	Nextflow	Pegasus	Swift	Taverna	Triana
Workflow Execution Models															
Sequential	✔	✔	✔	✘	✘	✔	✔	✔	✔	✔	✘	✔	✔	✔	✔
Concurrent	✘	✘	✘	✔	✔	✘	✘	✘	✘	✘	✔	✘	✔	✘	✘
Iterative	✘	✘	✘	✘	✘	✘	✘	✘	✘	✔	✔	✘	✔	✔	✘
Tightly coupled	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔
External steering	✘	✘	✘	✘	✘	✘	✘	✘	✘	✔	✘	✘	✘	✘	✘
Heterogeneous Computing Environments															
Co-location	✘	✘	✘	✔	✔	✔	✘	✘	✘	✘	✔	✔	✔	✘	✘
External location	✘	✔	✔	✘	✘	✘	✔	✔	✔	✔	✘	✔	✔	✔	✔
In situ	✔	✘	✘	✘	✘	✘	✘	✘	✘	✘	✘	✘	✘	✘	✘
Data Access Methods															
Memory	✔	✘	✘	✔	✔	✔	✘	✘	✘	✘	✔	✔	✔	✘	✘
Messages	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔
Local disk	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔
Shared file system	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔
Object store	✘	✘	✘	✘	✘	✘	✔	✘	✘	✘	✘	✔	✘	✔	✘
Other remote storage	✔	✘	✘	✘	✘	✘	✔	✘	✘	✘	✘	✔	✔	✔	✘

A characterization of workflow management systems for extreme-scale applications

2. How to select a WMS ?

Key Factors to Consider

- Several WMS solve same general problems
  - but differ in specific approach
- A few categories to think :
  - Interface: how are workflows constructed?
  - Workload: what does your workflow look like?
  - Community: what domains does the tool focus on?
  - Task-Flow vs Data-Flow;

Interface

- How does a user construct workflows?
  - Graphical: like assembling a flow chart
  - Scripting: use a workflow tool-specific scripting language to describe workflow
  - API: use a common programming language with a tool-provided API to describe workflow
- Which is best depends on your application
  - Graphical can be unwieldy with many tasks
  - Scripting and API can require more initial investment
  - Some WMS support multiple approaches

Workload

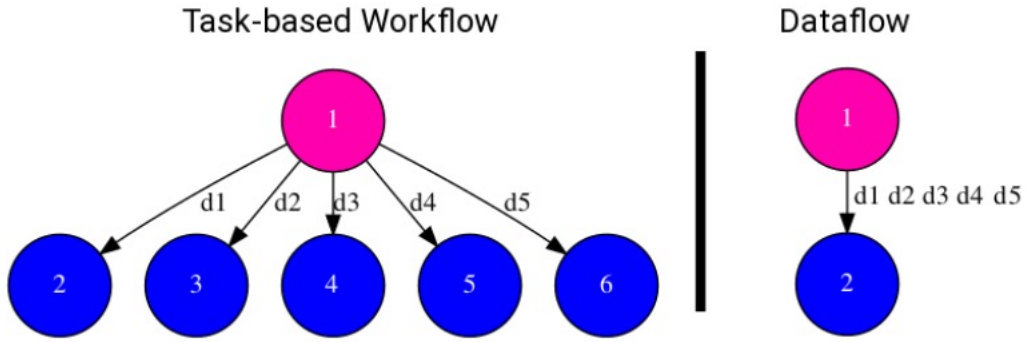
- What kind of workflow are you running?
  - Many vs. few tasks
  - Short vs. long
  - Dynamic vs. static
  - Loops vs. directed acyclic graph
- Different tools are targeted at different workload

Community

- What kinds of applications is the tool designed for?
- Some tools focus on certain science fields
  - Have specific paradigms or task types built-in
  - Workflow community will share science field
  - Less useful if not in the field or users of the provided tasks
- Some tools are more general
  - Open-ended, flexible
  - Less domain-specific community

Task-Flow vs Data-Flow

- Task-Flow:
  - Orchestrates isolated tasks processing data in sequence, based on data dependencies.
  - Ideal for structured, sequential processing where each task must complete before the next starts.
- Data-Flow:
  - Manages tasks for continuous data receipt and production;
  - Enables real-time data processing and inter-task communication without waiting for task completions.



- Key Difference:
  - Task-Flow focuses on sequential, dependent task execution, while Data-Flow emphasizes ongoing, real-time interaction between tasks

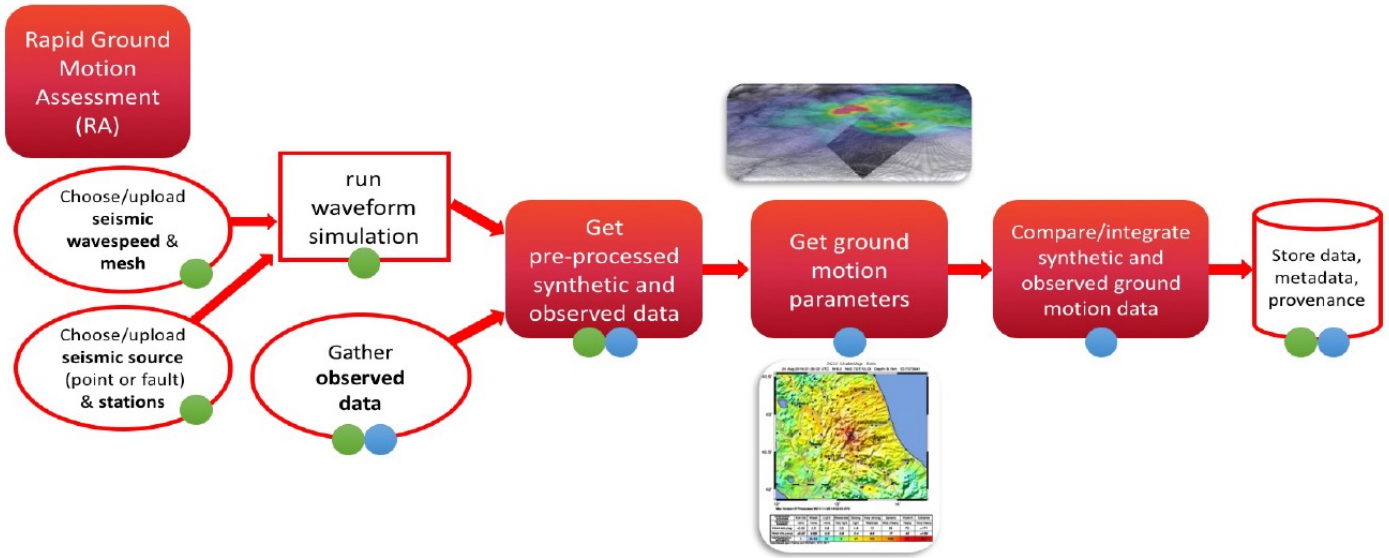
Task-Flow vs Data-Flow

dispel4py

Common Workflow Language

Real Examples – Rapid Assessment (RA)

- Rapid assessment (RA) of earthquakes' impact, and emergency response
  - Build dispel4py workflows to represent each part of the RA
    - Each part of RA follows a Data-Flow pattern
    - The full RA follows a Task-Flow pattern
  - Use CWL to connect RA dispel4py workflows



Real Examples – Internal Extinction (IE)

- Calculating the Internal Extinction of Galaxies
  - Crucial for determining a galaxy's optical luminosity
  - Build the full workflow in dispel4py
  - Each task/step in IE follows a Data-Flow pattern