MESHCHERYAKOV LABORATORY of INFORMATION TECHNOLOGIES

Workload Management System Development for SPD Online Filter

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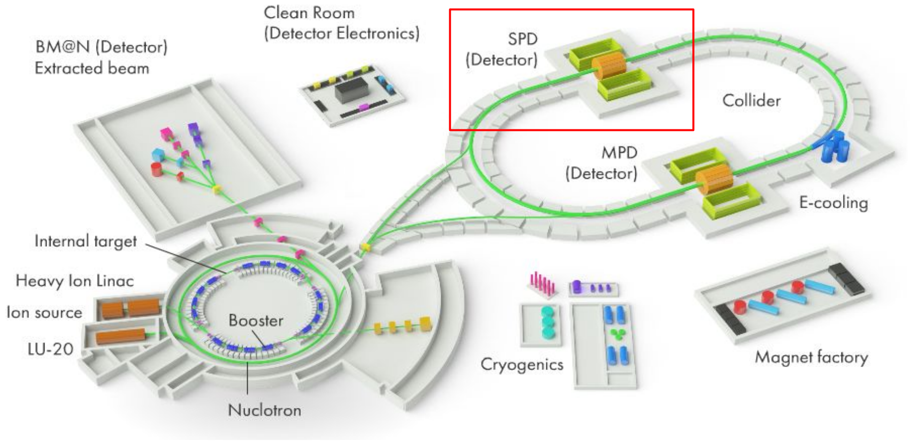
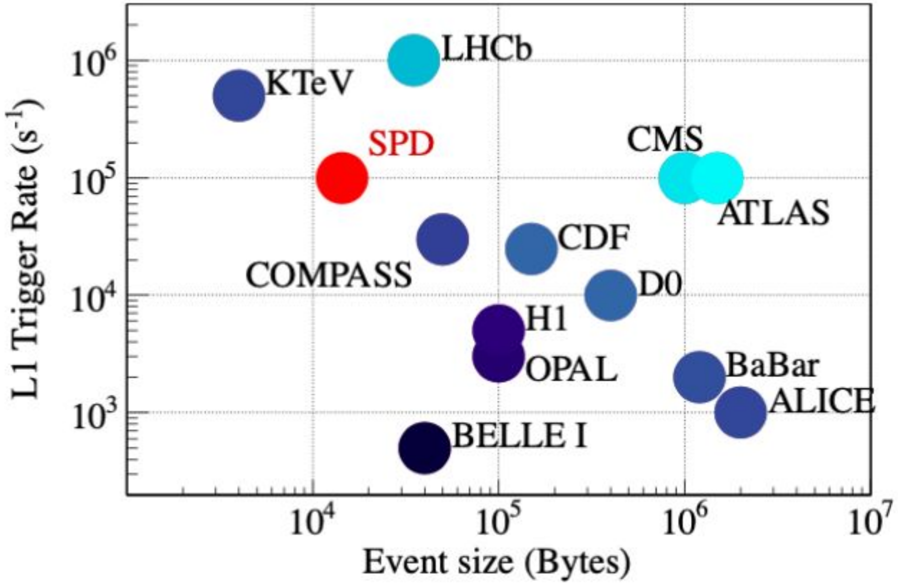
SPD experiment at NICA collider

The SPD detector (Spin Physics Detector) is one of the NICA infrastructure projects designed to study the spin and momentum of gluons and their distribution.



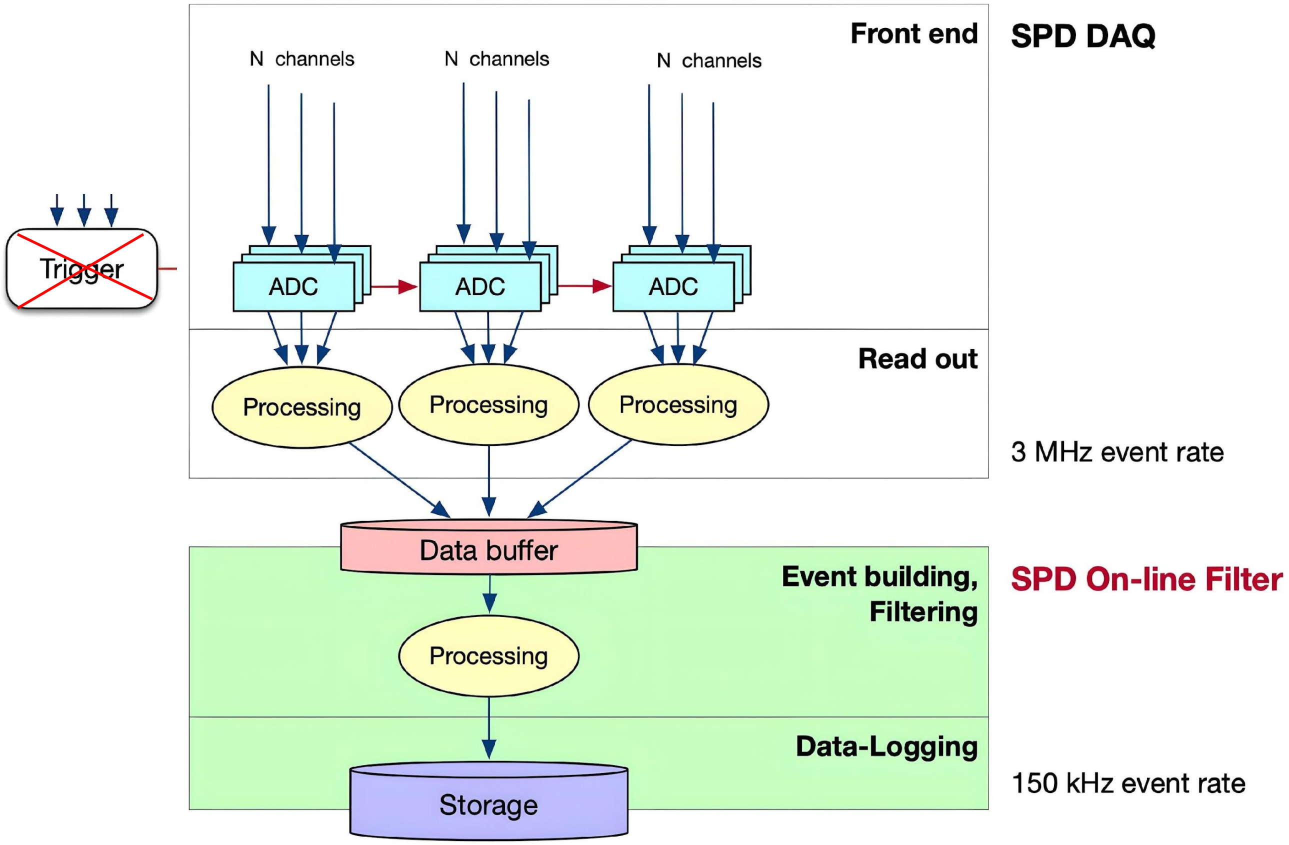
- Polarized proton and deuteron beams
- Collision energy up to 27 GeV
- luminosity up to 10^{32} cm^{-2} s^{-1}
- Bunch crossing every 80 ns = crossing rate 12.5 MHz

- Number of registration channels in SPD ~ 500000
- ~ 3 MHz event rate (at max luminosity) = pileups
  - ~ 20 GB/s (or 200PB/year) “raw” data
- Physics signal selection requires momentum and vertex reconstruction
  - => no simple trigger is possible

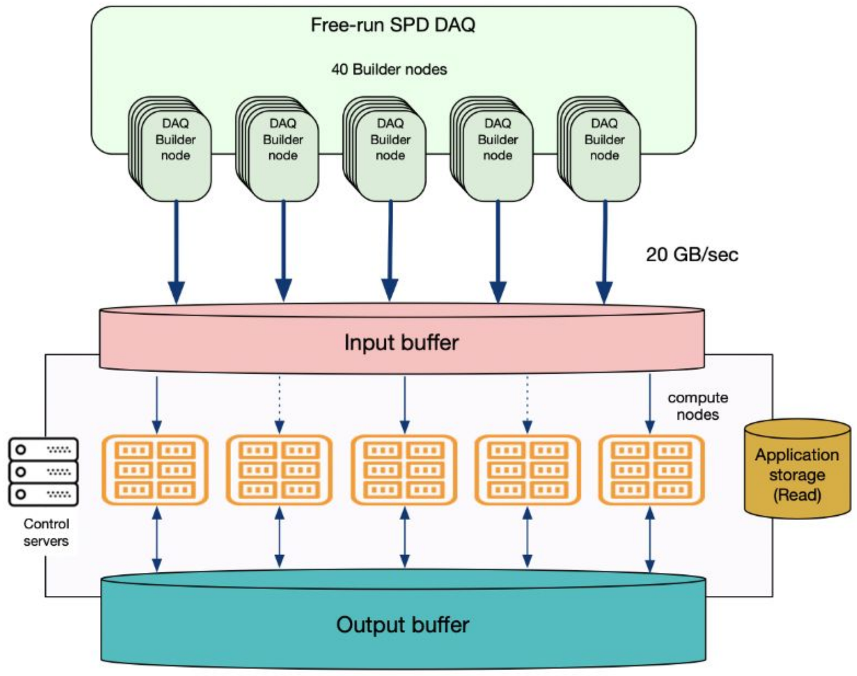


Triggerless DAQ

Triggerless DAQ means that the output of the system is not a set of raw events, but a set of signals from sub-detectors organized into time slices.



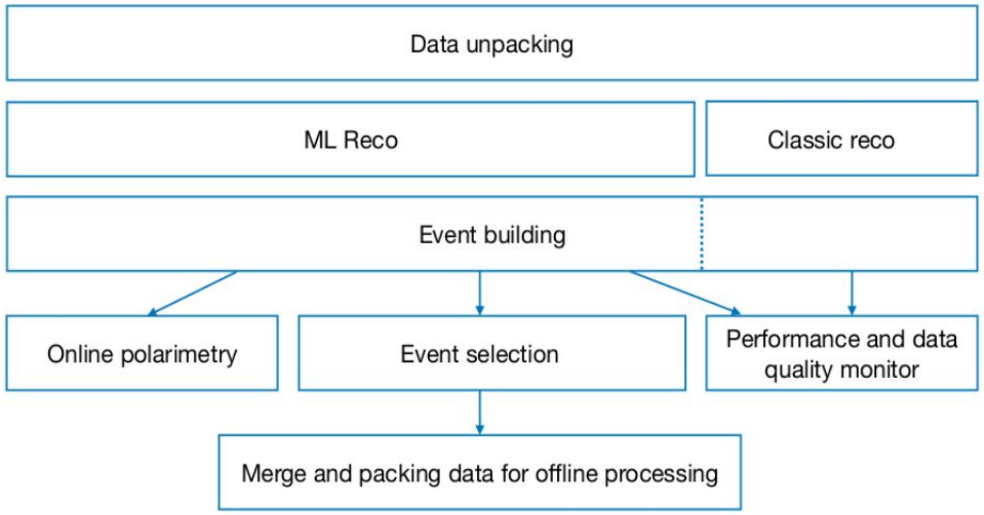
«triggerless» DAQ



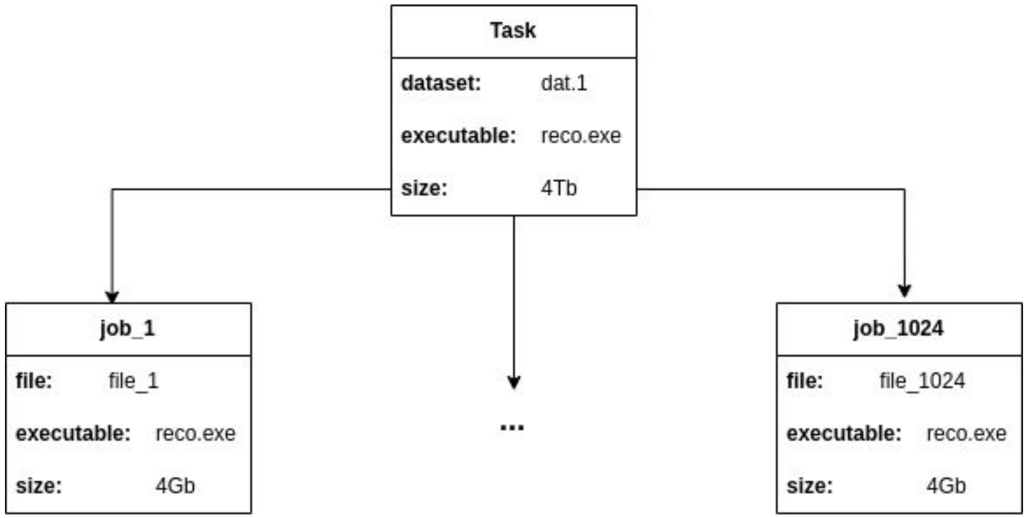
- ➢ DAQ provide data organized in time frames which placed in **files** with reasonable size (a few GB).
- ➢ Each of these file may be processed independently as a part of top-level **workflow chain**.
- ➢ No needs to exchange of any information during handling of each initial file, but results of may be used as input for next step of processing.

High-throughput computing

- **HTC** is defined as a type of computing that simultaneously executes numerous simple and computationally independent jobs to perform a data processing task.
- Since each data element can be processed simultaneously, this can be applied to data aggregated by a data acquisition system (DAQ).
- To ensure efficient utilization of computational resources, data processing should be multi-stage:
  - One stage of processing → **task**
  - Processing a block of data (file) → **job**



Data processing work chain example

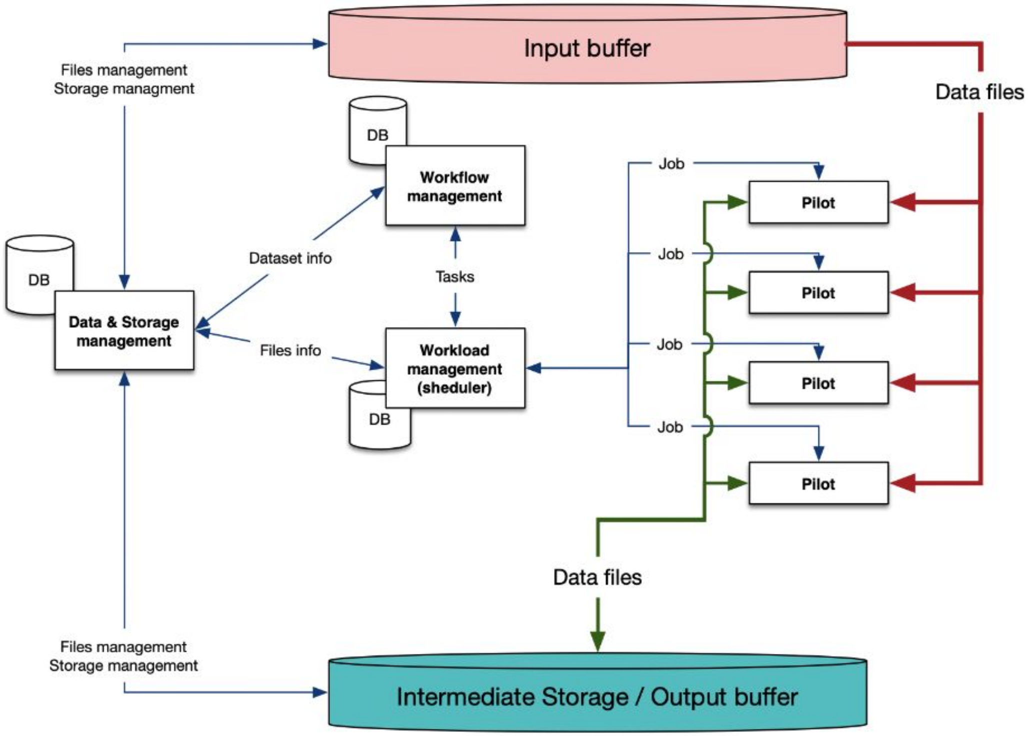


Task-job relationship

SPD Online Filter as a middleware software

«SPD OnLine filter» – hardware and software complex providing multi-stage high-throughput processing and filtering of data for SPD detector.

- **Data management system (one PhD student and one master student)**
  - Data lifecycle support (data catalog, consistency check, cleanup, storage);
- **Workflow Management System (master student)**
  - Define and execute processing chains by generating the required number of computational tasks;
- **Workload management system:**
  - Create the required number of processing jobs to perform the task;
  - Control job execution through pilots working on compute nodes;



Architecture of SPD Online Filter

Workload management system requirements

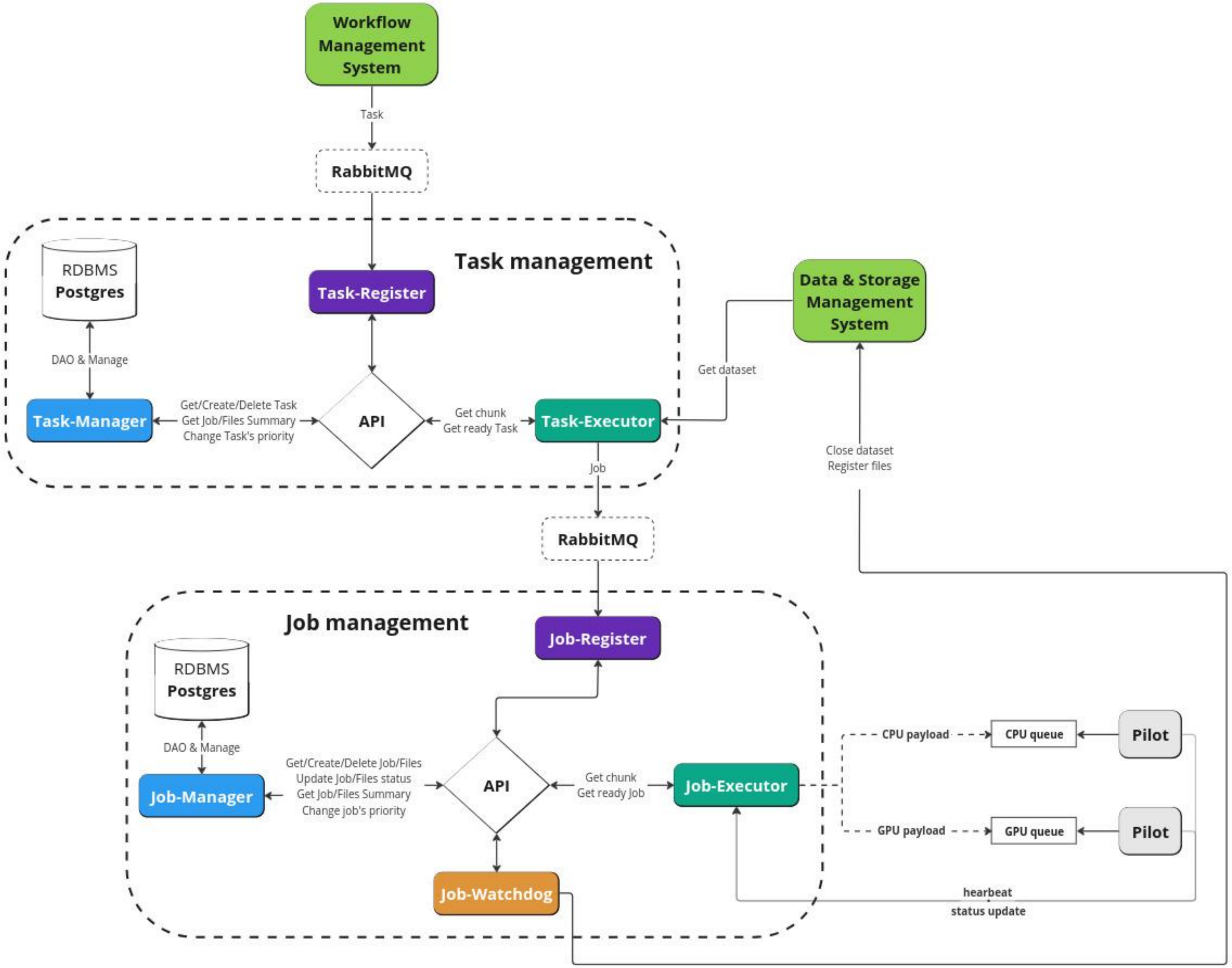
The key requirement - systems must meet the **high-throughput paradigm**.

- ❑ **Task registration**: formalized task description, including job options and required metadata registration;
- ❑ **Jobs definition**: generation of required number of jobs to perform task by controlled loading of available computing resources;
- ❑ **Jobs execution management**: continuous job state monitoring by communication with pilot, job retries in case of failures, job execution termination;
- ❑ **Consistency control**: control of the consistency of information in relation to the tasks, files and jobs;
- ❑ **Scheduling:** implementing a scheduling principle for task/job distribution;

Forming jobs based on dataset contents, one file per one job

Architecture and functionality of Workload Management System

- **task-manager** – implements both external and internal REST APIs. Responsible for registering tasks for processing, cancelling tasks, reporting on current output files and tasks in the system.
- **task-executor** – responsible for forming jobs in the system by dataset contents.
- **job-manager** – accountable for storing jobs and files metadata, as well as providing a REST API for the executed jobs.
- **job-executor** – responsible for distribution of jobs to pilot applications, updating the status of jobs
- **pilot** – responsible for running jobs on compute nodes, organizing their execution, and communicating various information about their progress and status.



SPD Workload Management System High Level Architecture

Pilot Agent

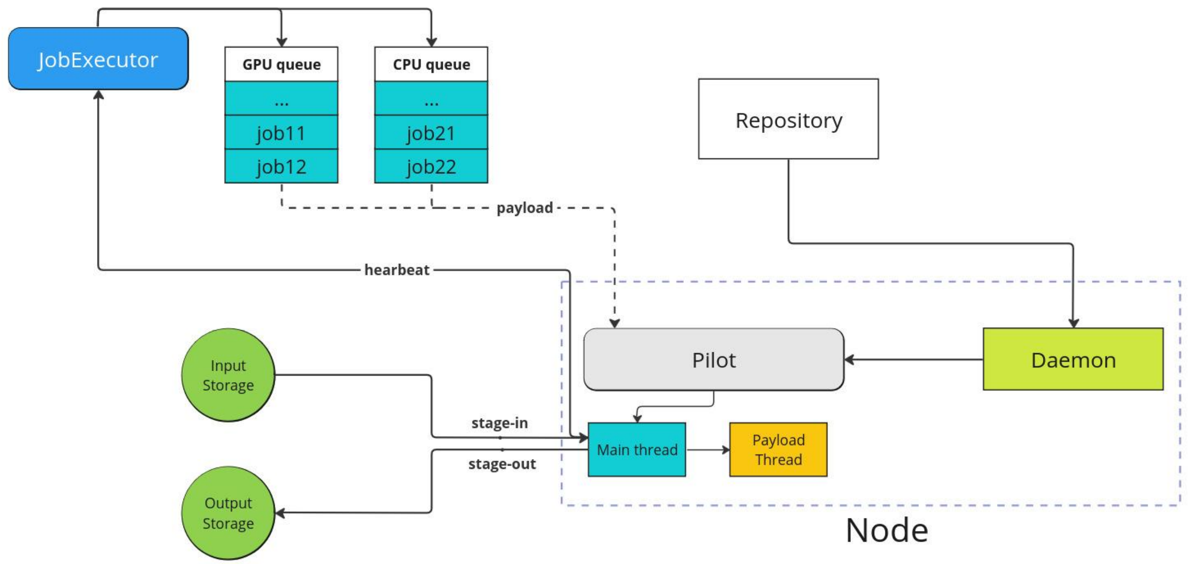
- The agent application is deployed on a compute node and consists of the following two components: a UNIX daemon and the pilot itself.
- The UNIX daemon's objective is to run the next pilot by downloading an up-to-date version from the repository.
- Pilot itself is a multi-threaded Python application responsible for
  - Receiving and validating jobs from the message broker;
  - Downloading input files for the payload stage and uploading the result files to the output storage;
  - Launching a subprocess to execute a payload (decoding DAQ format, track recognition algorithm, etc.)
  - Keeping the upstream system informed of the current status of the payload and the pilot itself via heartbeat/status updates during each phase of pilot execution;

Two types of nodes:

- Multi-CPU
- Multi-CPU + GPU

Two communication channels:

- HTTP (aiohttp)
- AMQP (message broker - RabbitMQ)

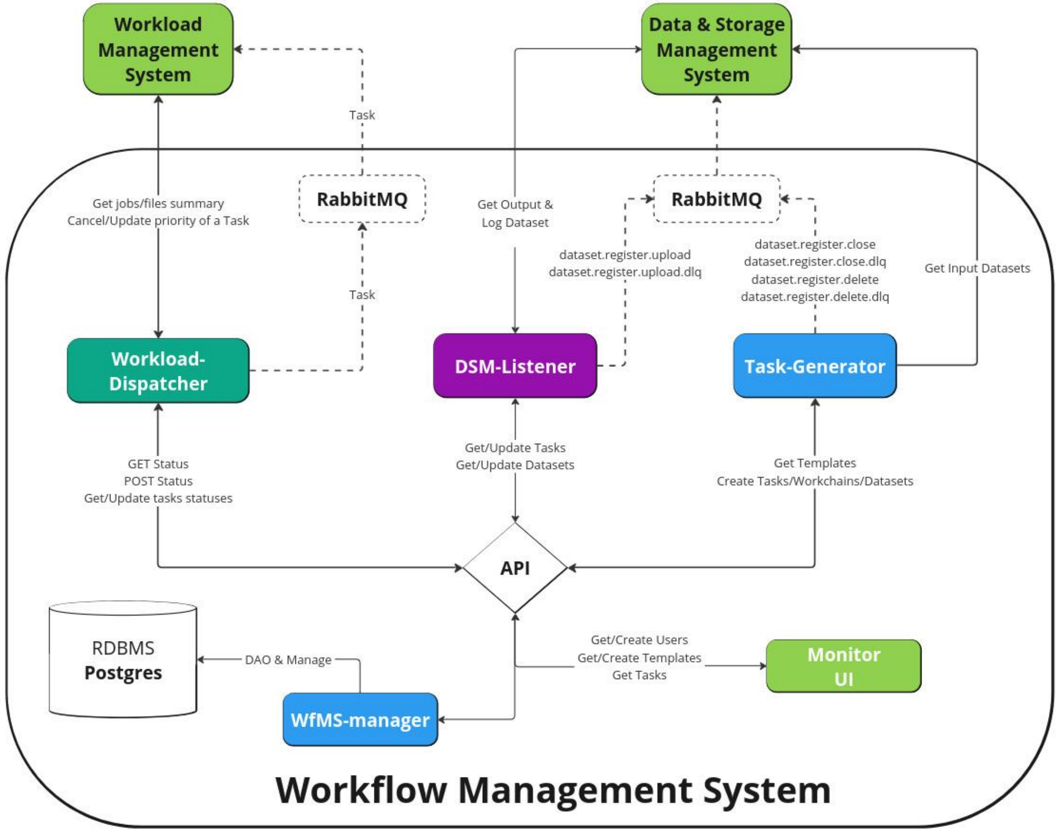


- ✓ A detailed job status model has been described;
- ✓ Error codes introduced;
- ✓ Pilot ran through all stages of the job execution (**D**irected **A**cyclic **G**raph);
- ✓ Pilot at this stage runs a script that does a basic hash compute;
- ✓ UNIX Daemon is implemented and currently running;

Interaction with Workflow Management System

The following interaction scenarios have been identified with the Workflow Management System

- Registration of a task for processing: **WfMS** passes the task description into the message queue;
- Summary of current intermediate properties of jobs/files in the system: aggregated information about the status of each job/file for further decision making;
- Task cancellation: based on the decision made on the **WfMS** (*too many errors occurring*) on operator side;
- Change priority of a task: is used to accelerate the rate at which the corresponding dataset is being processed;



Interaction with Data Management System

Routing Key	Msg	Algo
dataset.close	Dataset info • Dataset UID • File check list (file names)	Request the registered files in the dataset. If they match the checklist, set the status to **CLOSED**. Otherwise, return the messages back to the queue for deferred execution.
dataset.upload	Dataset UID	Marking dataset for uploading (**TO_UPLOAD**)
dataset.delete	Dataset UID	Marking dataset for deletion (**TO_DELETE**)

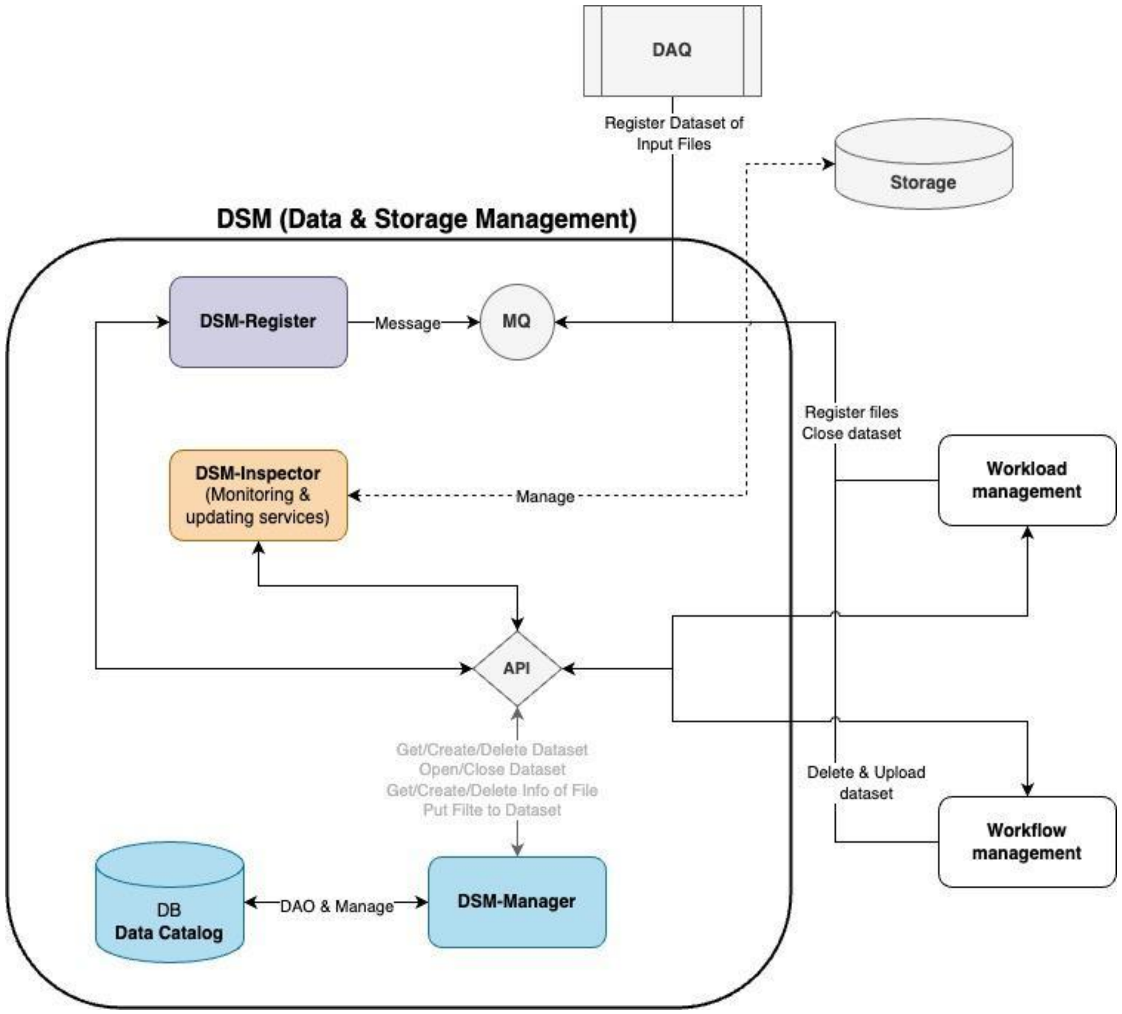
Signature and algorithm of message receiving gateways for the **dsm-register** service

Within a **Workload Management System**, there are several scenarios for interacting with the data management system:

➢ Obtain information about dataset contents for forming jobs from **DSM-Manager (Data Catalog REST API)**

➢ Register files in datasets after executing payload on compute node – **DSM-Register (Data Registration)**

➢ Close dataset after cancellation or sufficient number of successfully processed files – **DSM-Register***



Architecture of Data Management

Tereschenko, D., Ponomarev, E., Oleynik, D. *et al.* SPD On-Line Filter: Workflow and Data Management Systems. *Phys. Part. Nuclei* **55**, 603–605 (2024).

Database design

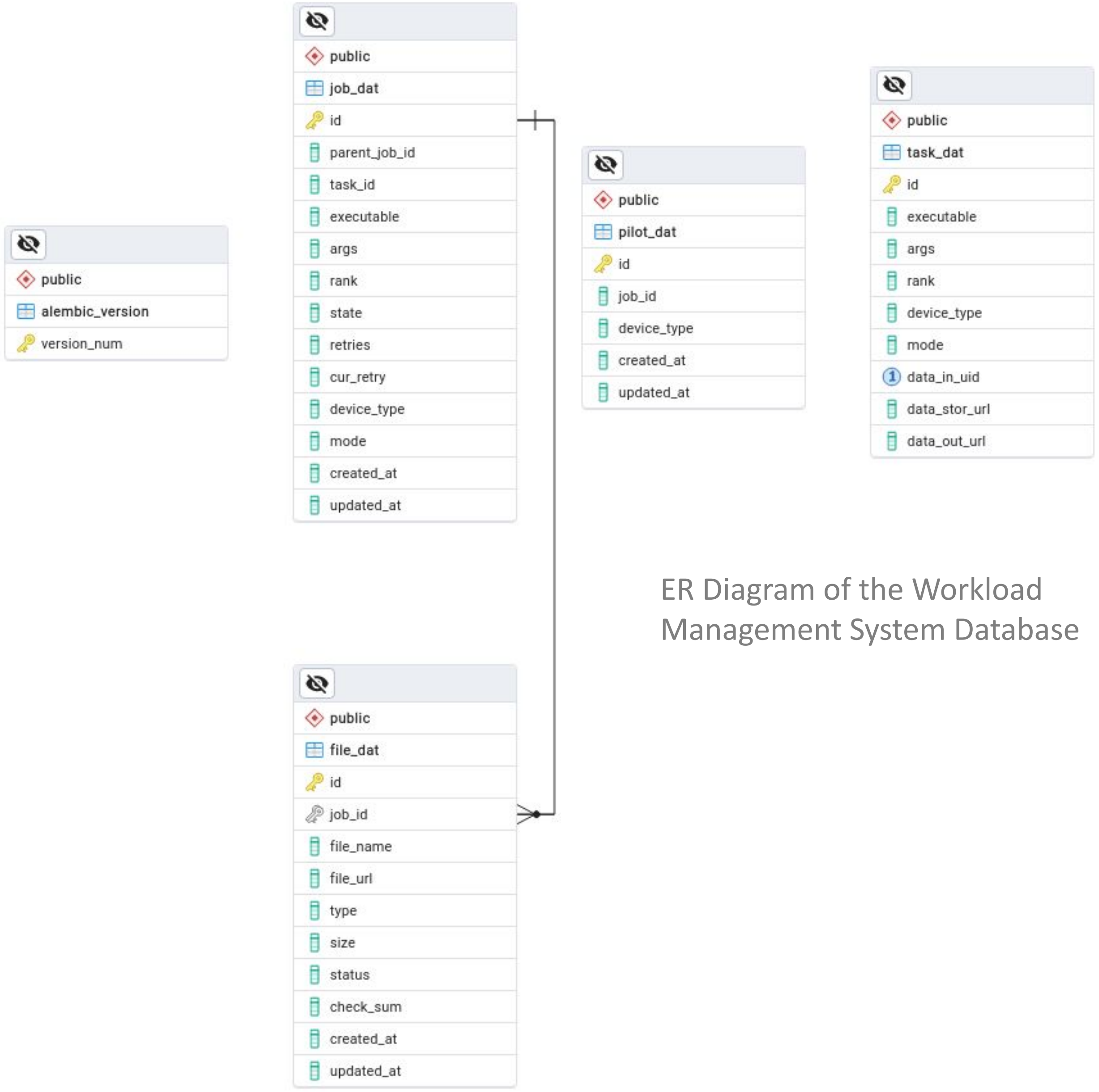
RDBMS - PostgreSQL 16

Tables:

- **alembic_version** – managing and tracking database schema changes
- **file_dat** – a directory specifying the output files and logs generated on the pilot
- **job_dat** – jobs currently being processed in the system
- **task_dat** – current tasks in the system

Extra mechanisms:

- **Indexes** – on filter fields for optimization of operations (B-tree);
- **Procedures** – task and job generation for test purposes;
- **Triggers** – rank update logic;
- **Decomposition** – single database per microservice (Postgres in Docker initially)



ER Diagram of the Workload Management System Database

Tech stack

Common	Frameworks
➢ Python 3.12 ➢ docker compose - running multi-container applications	➢ aio-pika (RabbitMQ + asyncio) - asynchronous API with RabbitMQ ➢ FastAPI + uvicorn
DB	**Extra**
➢ PostgreSQL - RDBMS ➢ Alembic (Migration) ➢ SQLAlchemy 2.0 ➢ asyncpg - Postgres DBAPI	➢ aiohttp - asynchronous HTTP client/server framework ➢ Pydantic - validate and serialize data schemes ➢ pytest-asyncio - test purposes

Current Status

Design of services:

- ✓ Designed and implemented a list of required REST API methods and their signatures;
- ✓ Implemented a mechanism for declaring the data model in the database based on ORM and migration scripts;
- ✓ Configured CD tools (build and deployment) on the JINR LIT infrastructure;
- ✓ Designed inter-service interaction scenarios – defined API contracts;
- ✓ Designed Pilot internal architecture;
- ✓ Workload Management System - Pilot Interaction Models in Finite State Machine.

Prototype of services:

- ✓ Most microservices implemented;
- ✓ Job management subsystem is the most advanced: most interactions implemented and being tested;
- ✓ Task partitioning is being implemented;
- ✓ Pilot and Pilot Daemon is currently working;
- ✓ Pilot handles all stages of job execution on the given workload.

Next major steps

- **Task processing**
  - Execute the entire workchain set up on the level of **WfMS**.
- **Middleware and applied software integration**
  - Requires prototyped applied software and simulated data.
- **Logging**
  - Currently, each microservice logs are mapped to the host via a shared file system between Docker and the host.
  - Ideally – **ELK** (*Elastic-Logstash-Kibana*) stack to build a log analysis platform.
- **Configuration**
  - Consider to centralize some of the shared configurations across multiple services (*Consul, Etcd*).
- **Documentation**
  - Given the increasing complexity of the internal logic of the software, it is necessary to document each step of the development.
- **Metrics and monitoring**
  - For example, service query-per-second, API responsiveness, service latency etc. (*InfluxDB, Prometheus, Graphana*)

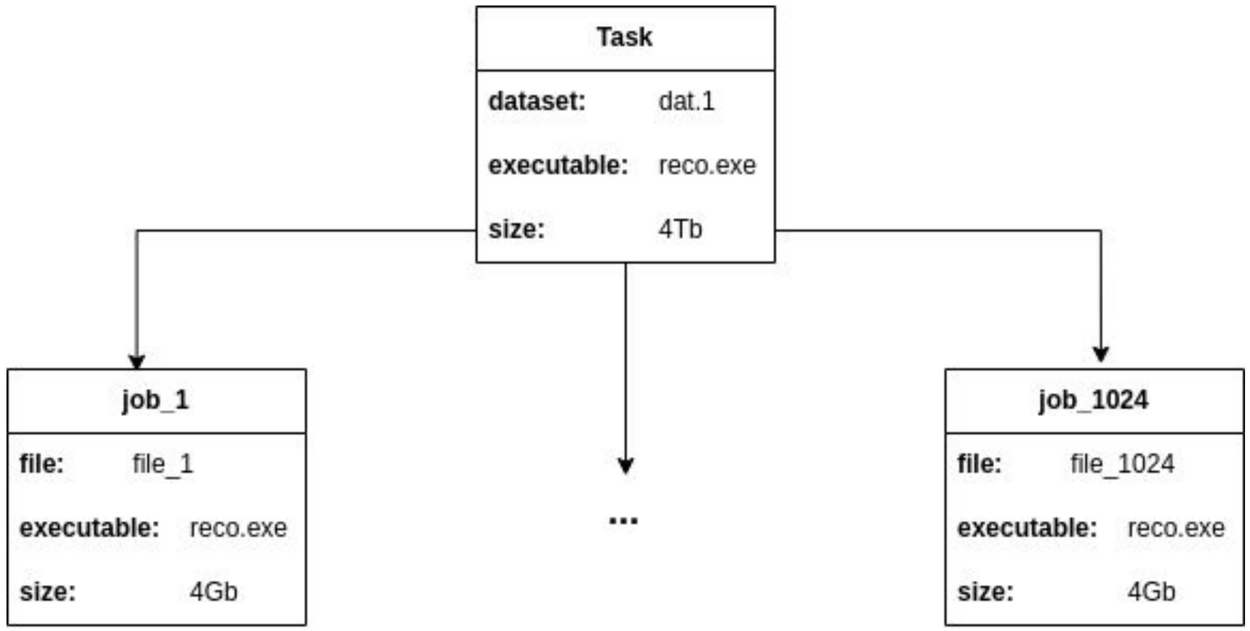
Thank you for your attention!

Backup slides

Task and job definition

- ➢ A **task** is a workload unit responsible for processing a block of homogeneous data - **dataset**.
- ➢ A processing request is a set of input data, which may consist of multiple files, and a handler.
- ➢ The criterion for the completion of the task is the processing of the entire block of data.
- ➢ The **Workflow Management System** is responsible for defining and executing workflows, as well as defining a processing request, which is a **task**.

- ➢ A **job** (payload) is a unit of work that processes a unit of data (**file**).
- ➢ The unit responsible for processing a single **file** in terms of workload is called a **job**.
- ➢ The **Workload Management System** is responsible for generating **jobs**, sending them to compute nodes, and executing them.

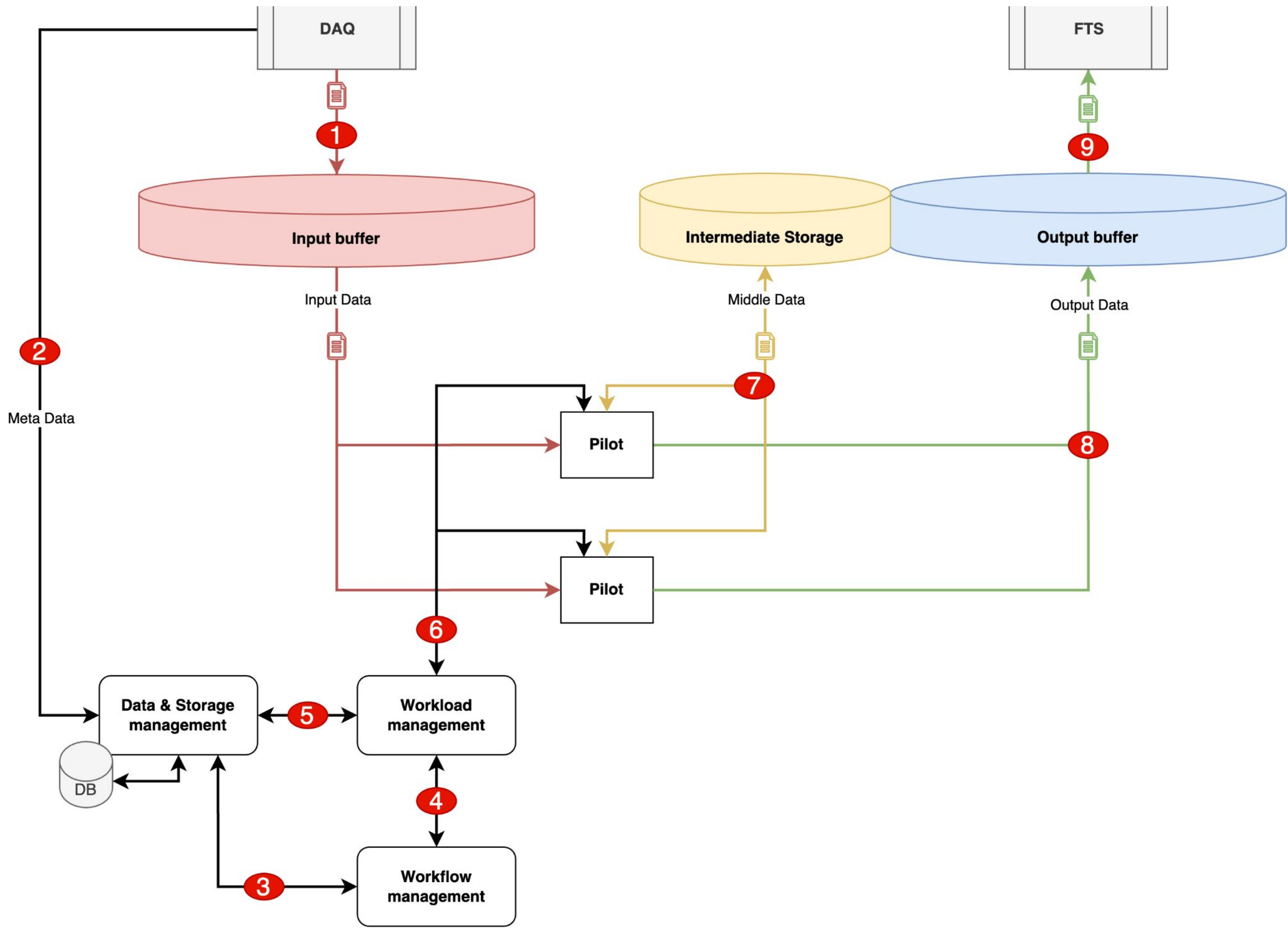


Task-job relationship

Dataflow and data processing concept

Main data streams:

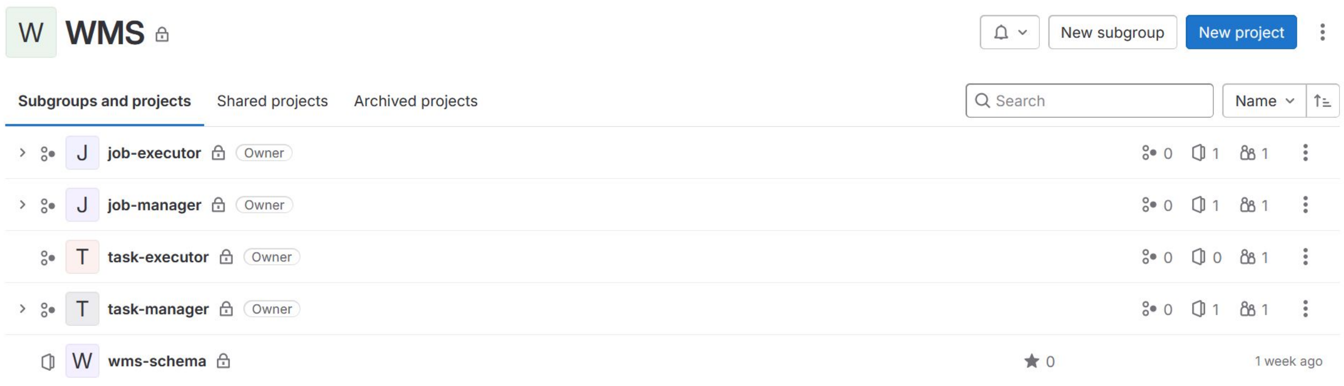
- SPD DAQs, after dividing sensor signals into time blocks, send data to the SPD Online Filter input buffer as files of a consistent size.
- The workflow management system creates and deletes intermediate and final data sets
- The **workload management system** “populates” the data sets with information about the resulting files
- At each stage of data processing, pilots will read and write files to storage and create secondary data

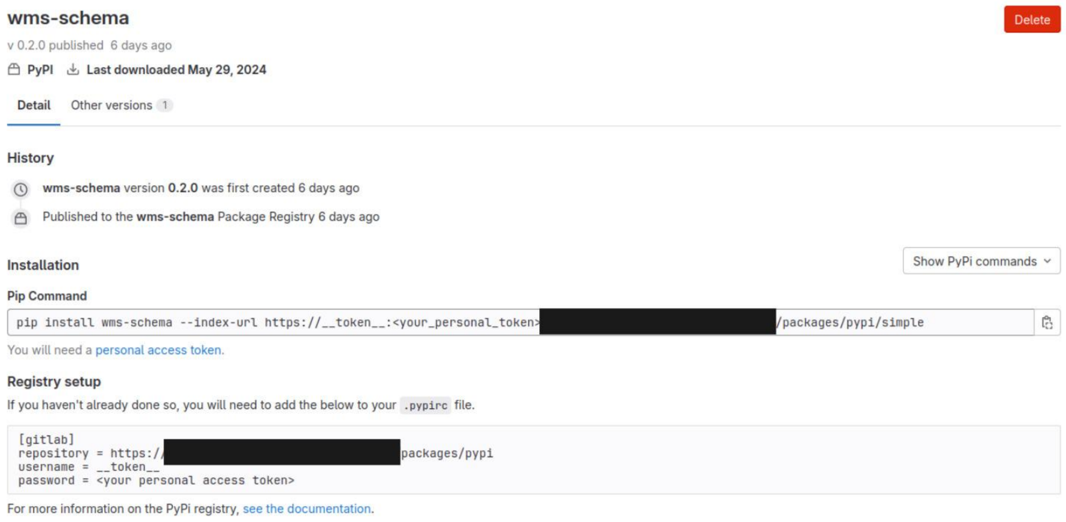


Modularization: deploying and using own packages

Following tools are used:

- ❖ Poetry
  - ➢ Particularly good at handling complex dependency trees and ensuring that the different modules can integrate with each other without version conflicts
- ❖ Python packages
  - ➢ Separate GitLab repositories for each package
  - ➢ Poetry for packaging and dependency management
- ❖ Gitlab
  - ➢ *Access Tokens* used as kind of credentials for scripts and other tools
  - ➢ CI/CD for automate testing and building

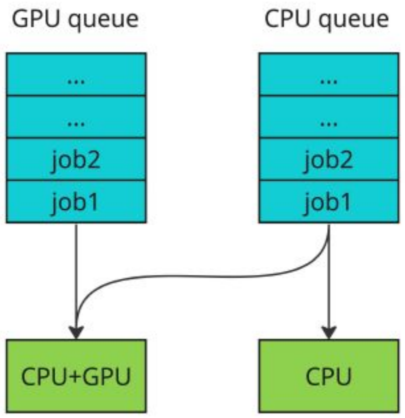


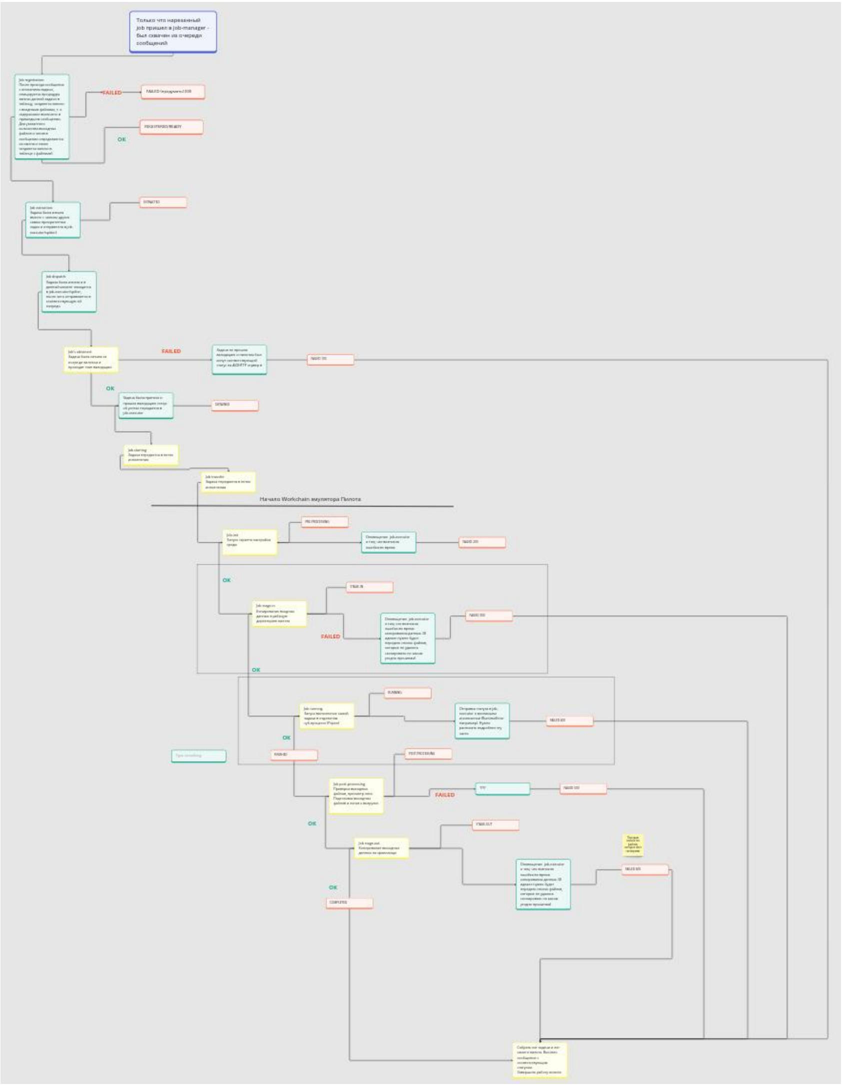


wms-schema is a package that contains a scheme for task and job data that is used in almost every other service

Interaction with the Pilot Agent

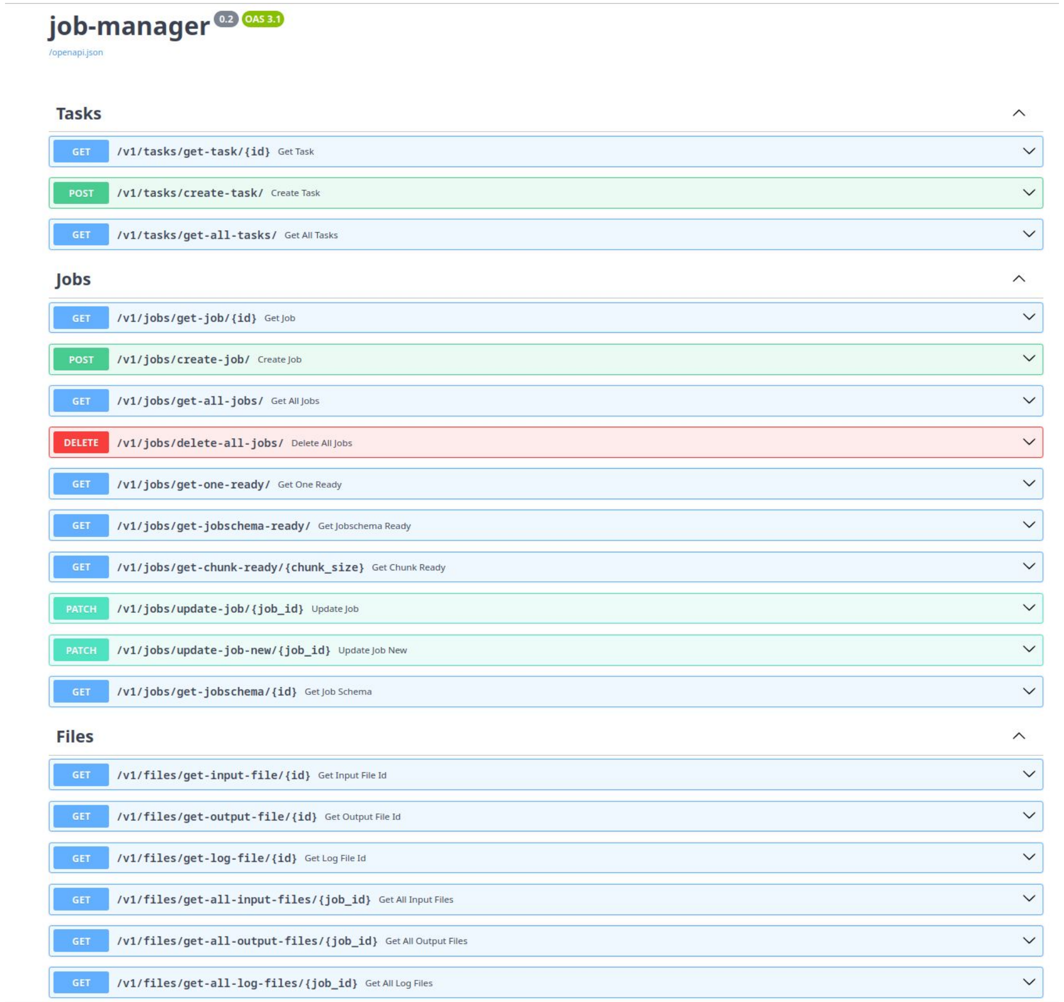
- Pilot has a series of prepossessing stages before running a job itself:
  a. start logging
  b. read configuration
  c. getting a job from message queue
  d. validation
- After those steps the Pilot launches another thread where it does
  a. environment setup script
  b. copying files locally from the input storage
  c. starts execution of a job itself in a separate sub-process
  d. analysis of the result of a job
  e. copying output data and logs to storage
  f. sends regular messages to **WMS**
  g. cleaning up the local environment
- Pilot sends status-update message at any point of internal changes
- **WMS** may terminate the job if the corresponding task is cancelled or if an error occurs.



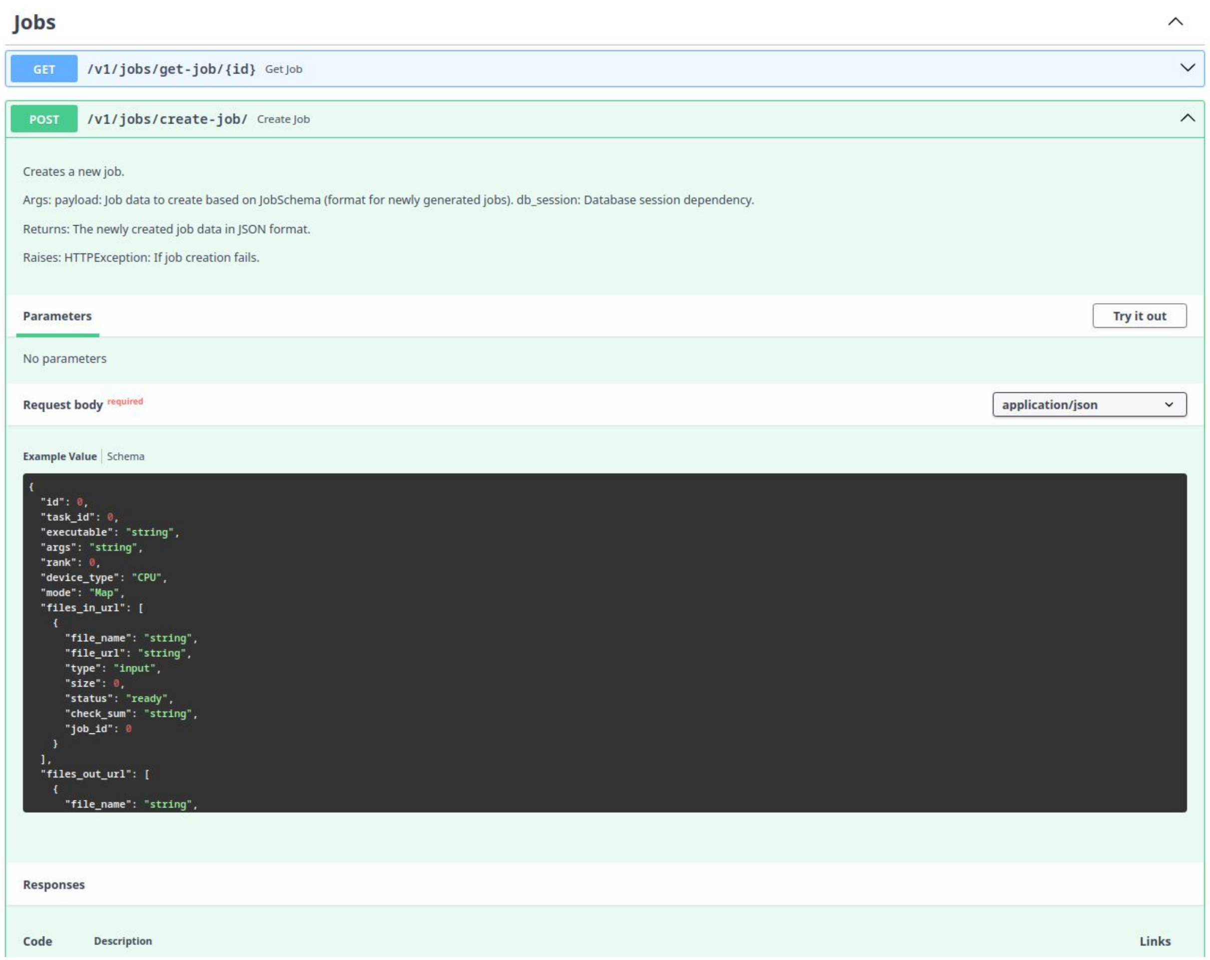


Prototyping Job-Manager (API)

- The chosen framework for building the service is FastAPI + Uvicorn asynchronous framework
- A basic set of CRUD operations on data in the form of REST API is developed.
- API description autogeneration according to OpenAPI 3.0 specification is implemented (available in Swagger UI at <server address>/docs)



Swagger UI with job-manager service API description

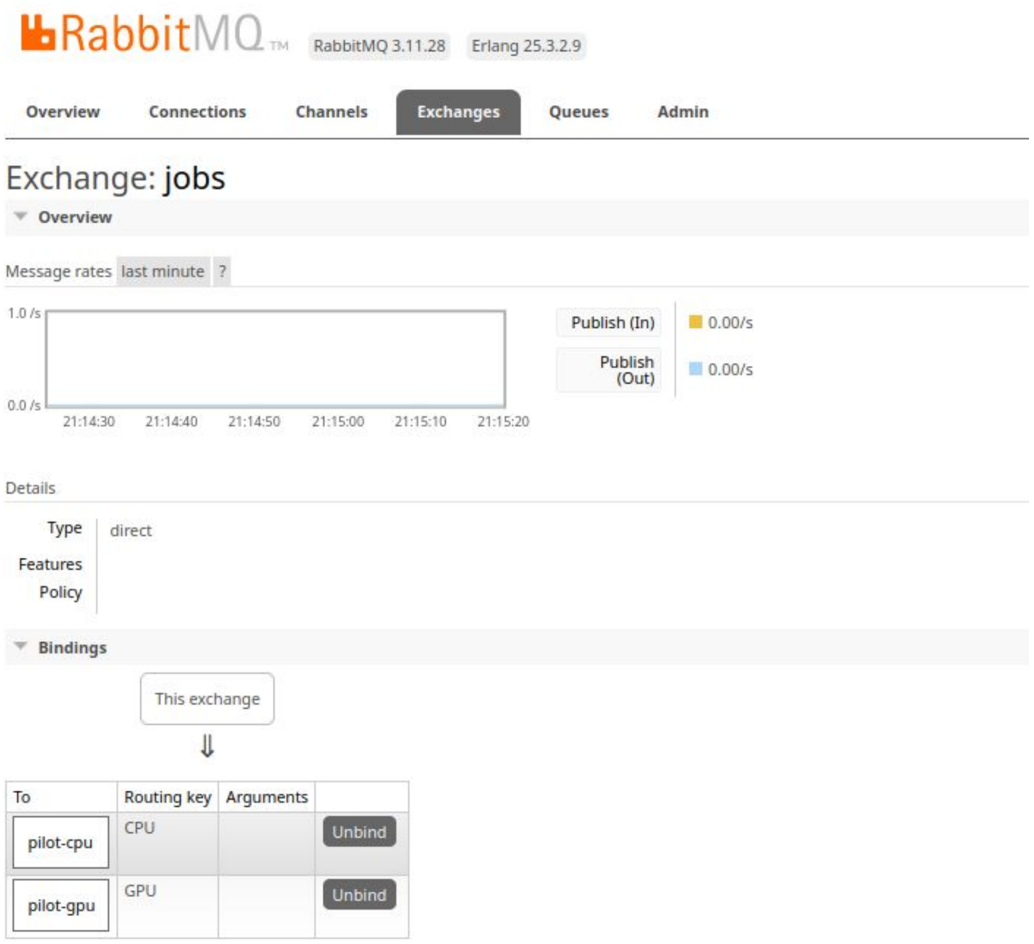


Example of a service call to post a new job

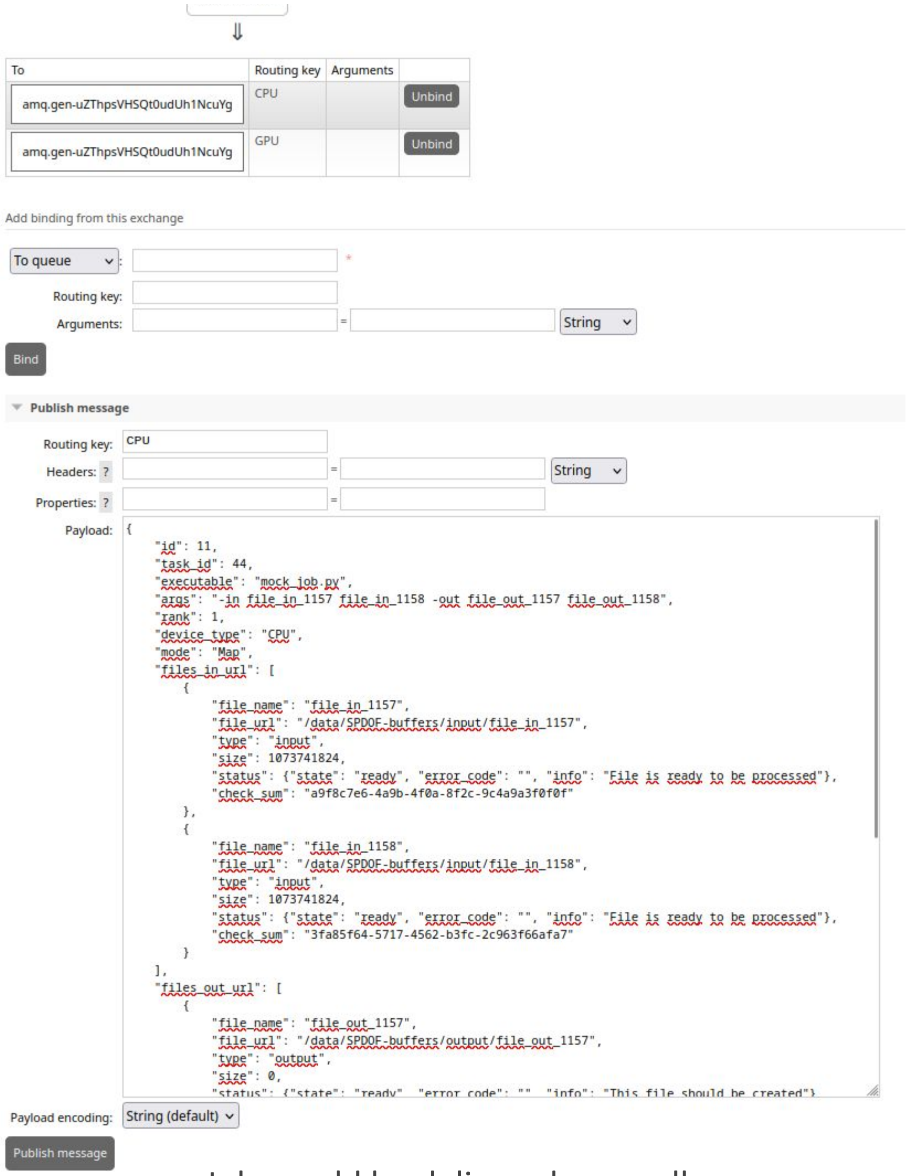
Prototyping Job-Executor - Pilot (RabbitMQ queues)

SPD NICA

- RabbitMQ is selected as the message broker
- Queues are defined using the declarative notation of the aio-pika tool
- At the start of the application their unfolding is performed



Configured RabbitMQ queues



Jobs could be delivered manually

Examples of Templates and Tasks

NICA SPD

- Registration and authorization
- Template and task output
- CWL template creation by user
- Preliminary validation and writing of CWL templates to the database

Template Manager Templates Tasks a@aaa.aaa Logout

Create template

template_id	name	inner_dataset_mask	description	status
1	template1	.test.	{"steps": {"decoding": {"run": {"class": "CommandLineTool", "baseCommand": "echo", "inputs": {"dataset_name": {"type": "string"}, "processing_program": {"type": "string"}, "processing_program_version": {"type": "string"}, "cable_map": {"type": "File"}, "input_params": {"type": "File"}}, "outputs": {"output_dataset": {"type": "File"}, "log_dataset": {"type": "File"}}}, "in": {"dataset_name": ".test.", "processing_program": "processing_program", "processing_program_version": "processing_program_version", "cable_map": "cable_map", "input_params": "input_params"}, "out": "[output_dataset, log_dataset]"}, "reconstruction": {"run": {"class": "CommandLineTool", "baseCommand": "echo", "inputs": {"dataset_name": {"type": "string"}, "processing_program": {"type": "string"}, "processing_program_version": {"type": "string"}, "cable_map": {"type": "File"}, "input_params": {"type": "File"}}, "outputs": {"output_dataset": {"type": "File"}, "log_dataset": {"type": "File"}}}, "in": {"dataset_name": ".test.", "processing_program": "processing_program", "processing_program_version": "processing_program_version", "cable_map": "cable_map", "input_params": "input_params"}, "out": "[output_dataset, log_dataset]"}}}	ACTUAL
2	template2	.test.	{"steps": {"decoding": {"run": {"class": "CommandLineTool", "baseCommand": "echo", "inputs": {"dataset_name": {"type": "string"}, "processing_program": {"type": "string"}, "processing_program_version": {"type": "string"}, "cable_map": {"type": "File"}, "input_params": {"type": "File"}}, "outputs": {"output_dataset": {"type": "File"}, "log_dataset": {"type": "File"}}}, "in": {"dataset_name": ".test.", "processing_program": "processing_program", "processing_program_version": "processing_program_version", "cable_map": "cable_map", "input_params": "input_params"}, "out": "[output_dataset, log_dataset]"}}}	ARCHIVED

Created template

Template Manager Templates Tasks a@aaa.aaa Logout

task_id	wflow_id	exec	args	rank	device	mode	retry	datas_in_id	datas_out_id	datas_log_id	status
11	6	processing_program	cable_map	1	CPU	map	5	26	27	28	IN_PROGRESS
12	6	processing_program	cable_map	1	CPU	map	5	27	29	30	IN_PROGRESS
13	7	processing_program	cable_map	1	CPU	map	5	31	32	33	IN_PROGRESS
14	7	processing_program	cable_map	1	CPU	map	5	32	34	35	IN_PROGRESS
15	8	processing_program	cable_map	1	CPU	map	5	36	37	38	IN_PROGRESS
16	8	processing_program	cable_map	1	CPU	map	5	37	39	40	IN_PROGRESS
17	9	processing_program	cable_map	1	CPU	map	5	41	42	43	IN_PROGRESS
18	9	processing_program	cable_map	1	CPU	map	5	42	44	45	IN_PROGRESS
19	10	processing_program	cable_map	1	CPU	map	5	46	47	48	IN_PROGRESS
20	10	processing_program	cable_map	1	CPU	map	5	47	49	50	IN_PROGRESS
21	11	processing_program	cable_map	1	CPU	map	5	51	52	53	IN_PROGRESS
22	11	processing_program	cable_map	1	CPU	map	5	52	54	55	IN_PROGRESS
23	12	processing_program	cable_map	1	CPU	map	5	56	57	58	IN_PROGRESS
24	12	processing_program	cable_map	1	CPU	map	5	57	59	60	IN_PROGRESS

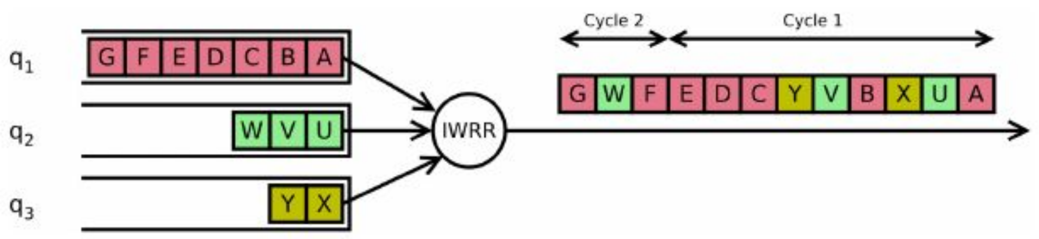
WfMS task description

R&D

- Jobs scheduling algorithm
- Partitioning of a task
  - Imagine a multitasking operating system.
  - Each dataset represents a process, and each record within a dataset is like a thread within that process.
  - The algorithm acts as the operating system's scheduler, allocating processing time to threads based on their priority.
- Chunk size and rank/priority of a job as a basic control unit:

$$rank_{i+1} = \alpha \times x_i + \beta \times y_i + \gamma \times rank_i$$

$$x_i - aging,\ y_i - retries$$



Interleaved Weighted round-robin

Algorithm 1 Task Scheduling Algorithm

```
Variables:
global_queue – global queue with tasks
dataset – array of datasets
N – number of datasets
rank_max – maximum task priority
heap – binary heap storing maximum task priorities
rank – array with task priorities
Algorithm:
initilize_datasets(dataset)
build_heap(rank)
while true do
    rank_max = heap.top()
    for r = 1 to rank_max do
        for i = 1 to N do
            if not dataset[i].chunk.empty() and rank[i] ≥ r then
                await dataset[i].chunk.cur_item
                update(dataset[i].chunk – ¿ cur_item)
            else if dataset[i].chunk.empty() then
                if dataset[i].chunk.cur_item then
                    dataset[i] = global_queue.head()
                end if
                update(rank[i])
                update(heap)
            end if
        end for
    end for
end while
```

Proposed task-partitioning algorithm