MOLGENIS EMX2 & HPC Job Orchestration — Design Proposal

Contents

1 Abstract

EMX2 is evolving to support heavy compute workloads (including AI) that cannot run inside the application stack and cannot be triggered via inbound connections into available HPC clusters. At the same time, EMX2 must remain the authoritative system of record for job state and artifact metadata, while HPC governance must retain control over scheduling and resource allocation. This creates a coordination problem across a strict trust boundary.

This document proposes an outbound-only execution bridge: the HPC head node polls EMX2 for work, claims jobs atomically, submits them to Slurm, and reports lifecycle transitions and artifacts back to EMX2.

EMX2 owns state and integrity; HPC owns execution and scheduling. The result is deterministic, auditable job orchestration without breaking institutional network constraints or governance boundaries.

2 Introduction

2.1 Motivation

Molgenis EMX2 is a metadata-driven platform for scientific data built around FAIR principles (findability, accessibility, interoperability and reusability). As the platform evolves to incorporate AI-backed enhancements — automated annotation, similarity search, inference pipelines — it needs the ability to offload compute-intensive workloads to GPU-enabled infrastructure that typically lives outside the application's own network.

This document proposes a protocol for bridging EMX2 with one or more HPC clusters managed by Slurm. The design addresses a specific institutional constraint: the HPC environment cannot accept inbound connections. All communication MUST be initiated from the HPC side.

The proposed architecture is an outbound-only job execution bridge. HPC workers poll EMX2 for work, claim jobs, execute them (inside Apptainer containers or via wrapper scripts), and report results — all without EMX2 needing to reach into the cluster.

2.2 Scope

This proposal covers worker registration and capability advertisement, job lifecycle management, artifact management (typed, content-addressed data objects for job inputs and outputs), and authentication across the trust boundary.

It does not cover job creation by end users (that is an EMX2 application concern), Slurm cluster administration, or artifact retention policy.

2.3 Terminology

Term	Meaning
Worker	A head node controller that registers with EMX2, polls for jobs, and submits them to Slurm.
Processor	A logical identifier for a type of workload (e.g. `text-embedding:v3`).
Profile	An abstract resource tier (e.g. `gpu-medium`) mapped to Slurm parameters on the HPC side.
Artifact	A typed, content-addressed data object tracked by the artifact registry.
Transition	A recorded state change on a job, created as a sub-resource of that job.

3 System Architecture

The system is divided into two trust domains connected by outbound HTTPS from the HPC environment. This section describes the proposed components in each domain and how they would interact.

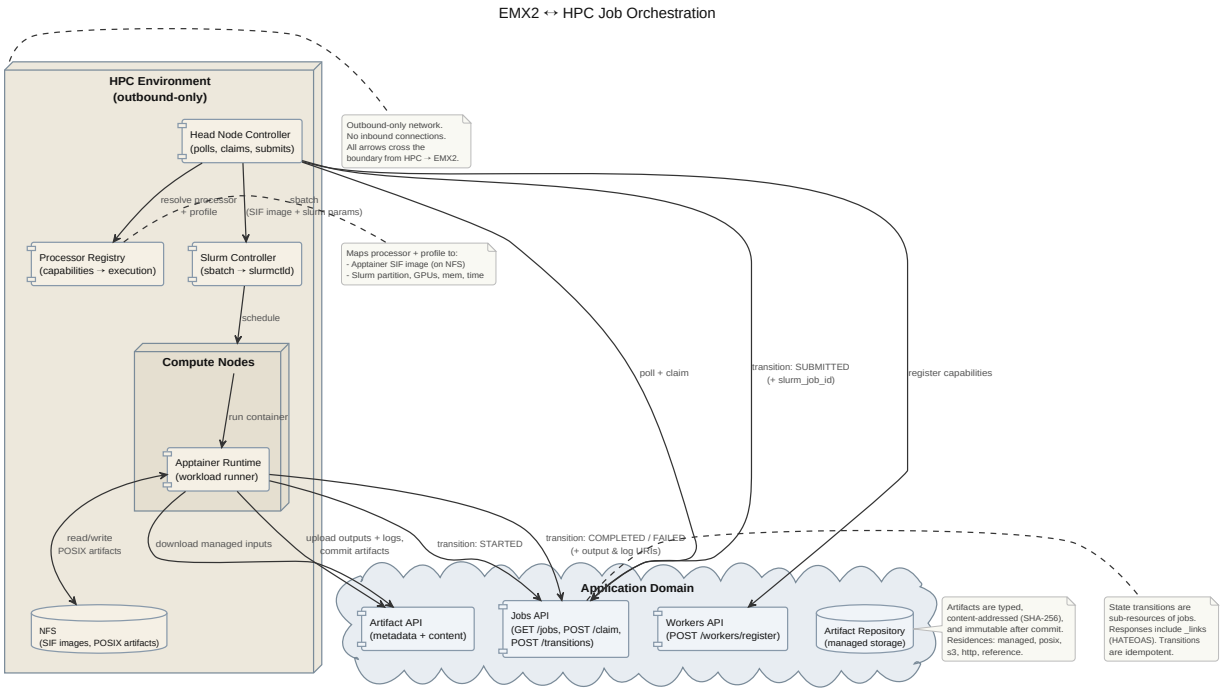


Figure 1: HPC Topology

3.1 EMX2 Application Domain

This proposal introduces three API surfaces within EMX2:

- **Workers API** — registration of head nodes and their capabilities.
- **Jobs API** — job listing, filtering by capability, atomic claiming, state transitions, and output artifact linking.
- **Artifact API** — lifecycle management (create/upload/commit), path-based file operations (PUT/GET/HEAD/DELETE), paginated file listing, and integrity verification. Exposes an S3-minimal surface for managed artifacts.

These would be backed by tables in the EMX2 `_SYSTEM_` schema (prefixed with `Hpc` to avoid collisions). The system tables would hold job state (including `output_artifact_id` foreign key to artifacts), worker registrations, capability advertisements, transition audit logs, artifact metadata, and artifact file content (stored in EMX2 FILE columns for managed residence). A Vue-based HPC dashboard would provide browser access to jobs, workers, and artifacts including direct file upload.

All endpoints would live under `/api/hpc/*` with a shared before-handler that validates protocol headers and (when configured) HMAC authentication. The health endpoint (`/api/hpc/health`) SHOULD be exempt from authentication.

3.2 HPC Environment

The HPC side consists of:

- **Head Node Controller** — a daemon that registers capabilities, polls for pending jobs, maps processor + profile to Slurm parameters, submits `sbatch`, and reports the result back to EMX2.
- **Slurm Controller** — the cluster's workload manager, unchanged from its standard role.
- **Apptainer Runtime / Wrapper Script** — executes the workload on a compute node, either inside an Apptainer (formerly Singularity) container or via a wrapper script executed directly on the host. The daemon would handle all communication with EMX2: staging input artifacts (symlink for posix, download for managed), monitoring Slurm job state, reading filesystem-based progress updates, uploading or registering output artifacts, and posting status transitions. The workload itself would have no direct EMX2 access — its only output channel is the filesystem (exit code, output files, and an optional `.hpc_progress.json` progress file).
- **NFS Shared Storage** — an NFS export mounted on the head node and all compute nodes. Stores Apptainer SIF images, POSIX-resident artifacts, and shared scratch data.
- **Local Scratch** — per-node temporary storage, discarded after job completion.

3.3 Separation of Responsibilities

Concern	Owner
Job registry, lifecycle state, artifact metadata, managed file storage	EMX2
Capability registration, job claiming, Slurm submission, artifact staging	Head Node Controller
Workload execution	Apptainer Runtime or Wrapper Script
Scheduling, resource allocation, node dispatch	Slurm Controller
Managed artifact binary content (FILE columns)	EMX2 Database
Shared data between jobs, POSIX-resident artifacts	NFS

3.4 Head Node Daemon

This proposal specifies the head node controller as a Python CLI (`emx2-hpc-daemon`), built on Click for argument parsing, httpx for HTTP communication, and subprocess for Slurm command invocation. It exposes four commands:

Command	Purpose
`run`	Start the daemon main loop (register → poll → claim → submit → monitor, repeating).
`once`	Run a single poll-claim-monitor cycle, then exit. Suitable for cron-based invocation.
`register`	Register the worker with EMX2 and exit.
`check`	Validate config, connectivity, and Slurm command availability.

Both `run` and `once` SHOULD accept a `--simulate` flag that walks jobs through all lifecycle states without invoking Slurm or creating working directories. In simulate mode, each poll cycle would advance tracked jobs

one step (CLAIMED → SUBMITTED → STARTED → COMPLETED), completing a full lifecycle in approximately three cycles.

The daemon SHOULD send periodic heartbeats (default: every 120 seconds) to keep the worker registration alive. On startup, it SHOULD recover tracking state for non-terminal jobs from a previous run. On SIGTERM/SIGINT, it SHOULD stop accepting new work and exit gracefully; Slurm jobs continue running independently and would be recovered on next startup.

During the monitor loop, the daemon SHOULD also check for a `.hpc_progress.json` file in each STARTED job's output directory. When the workload writes this file (with optional `phase`, `message`, and `progress` fields), the daemon reads it and relays the progress as a transition detail update to EMX2. This provides in-flight progress visibility without leaking any credentials into the job environment.

Configuration SHOULD be via a YAML file specifying EMX2 connection details, Slurm parameters, Apptainer settings, and profile-to-resource mappings.

4 End-to-End Protocol

The happy-path sequence proceeds in four phases (see Appendix B for the sequence diagram).

Phase 1 — Registration and job acquisition. The head node registers its capabilities with the Workers API, then polls the Jobs API for pending jobs that match its declared processors and profiles. When it finds one, it claims it. The claim MUST be atomic: if two workers try to claim the same job, only one succeeds.

Phase 2 — Input staging and Slurm submission. The head node stages input artifacts: for posix artifacts it symlinks the `file://` path into the job's input directory (zero-copy); for managed artifacts it downloads files via `GET /api/hpc/artifacts/{id}/files/{path}`. SHA-256 hashes MUST be verified after staging. The head node then maps the job's processor and profile to execution parameters — either an Apptainer SIF image or a wrapper script entrypoint — and a set of Slurm parameters, then submits via `sbatch`. It reports the Slurm job ID back to EMX2 as a SUBMITTED transition.

Phase 3 — Execution and monitoring. Slurm dispatches the job to a compute node, where it runs either inside an Apptainer container or as a wrapper script (see §5). The daemon monitors the job via `squeue`/`sacct` and posts a STARTED transition to EMX2 when execution begins. During execution, the daemon checks for a `.hpc_progress.json` file in the job's output directory and relays progress updates to EMX2 as transition detail updates. All EMX2 communication MUST be driven by the daemon — the workload itself has no direct access to EMX2.

Phase 4 — Output and completion. When the daemon detects job completion via Slurm, it creates an output artifact, uploads files (for managed residence) or registers the output directory path (for posix residence), and commits. It posts a COMPLETED transition with the `output_artifact_id` field linking the job to its output artifact. The artifact ID is stored as a foreign key on the job record, making outputs discoverable via GraphQL.

At every step, the client discovers what it can do next from hypermedia links in the response. If a transition is not legal in the current state, the corresponding link MUST be absent. Failure at any point results in a FAILED transition with a reason code (see Job Lifecycle, below).

4.1 Design Principles

The proposed architecture is deliberately minimal:

- **EMX2 is the system of record** for jobs, lifecycle state, and artifact metadata.
- **HPC is responsible for execution** via Slurm and Apptainer. EMX2 MUST NOT tell the cluster how to schedule.
- **Inputs and outputs are tracked as artifacts.** Jobs reference artifacts by ID. Content is accessed via the artifact file API (managed) or directly via `file://`, `s3://`, or `https://` URIs (external). Managed artifacts store binary content in EMX2; external artifacts store only metadata.
- **Workers declare capabilities; EMX2 assigns only compatible jobs.** There is no negotiation.
- **The API is resource-oriented.** State transitions are sub-resources of jobs. Responses include hypermedia links advertising legal next actions.
- **Everything is recoverable.** Transitions MUST be idempotent, timeouts detect stuck jobs, and the system converges to a consistent state after any single failure.

5 Processor and Execution Model

Jobs reference a logical processor identifier (e.g. `text-embedding:v3`) and an optional execution profile (e.g. `gpu-medium`). EMX2 MUST NOT encode cluster-specific scheduling parameters. Instead, the protocol proposes a hybrid model that separates **application intent** from **cluster policy**.

EMX2 specifies *what* to run — a processor identifier and a profile. The head node determines *how* — which SIF image, which Slurm partition, how many GPUs, how much memory, and what wall time.

For example, given a job requesting `text-embedding:v3` with profile `gpu-medium`, the head node would resolve this to:

```
text-embedding:v3 + gpu-medium
    → image: /nfs/images/text-embedding_v3.sif
    → partition: gpu
    → gpus: 1
    → cpus_per_task: 8
    → mem: 64G
    → time: 04:00:00
    → command: apptainer exec --nv /nfs/images/text-embedding_v3.sif ...
```

This mapping is maintained locally on the HPC system and MAY evolve independently of the protocol.

5.1 Wrapper Scripts (Entrypoint Mode)

Not all workloads fit the "run one container command" model. Multi-process orchestration, module loads, venv activation, and structured teardown require direct host access. For these cases, profiles MAY specify an `entrypoint` instead of (or alongside) `sif_image`.

When `entrypoint` is set, the batch script exports well-defined environment variables and `exec`s the wrapper script directly on the host:

```yaml
profiles:
  vtm-pipeline:gpu-large:
    entrypoint: /nfs/scripts/vtm-pipeline.sh
    partition: gpu
    cpus: 16
```

```
  memory: 128G
  time: "08:00:00"
```

The proposed wrapper script contract defines these environment variables:

- **`HPC_JOB_ID`** — the EMX2 job identifier.
- **`HPC_INPUT_DIR`** — directory containing staged input artifacts (read from here).
- **`HPC_OUTPUT_DIR`** — directory for output files (write results here).
- **`HPC_WORK_DIR`** — scratch working directory.
- **`HPC_PARAMETERS`** — JSON string with the full job parameters object.
- Any extra environment variables from the profile or job parameters.

The wrapper's responsibilities: read inputs from `HPC_INPUT_DIR`, write results to `HPC_OUTPUT_DIR`, and exit 0 on success. Optionally, write `.hpc_progress.json` to `HPC_OUTPUT_DIR` for in-flight progress reporting. The wrapper MUST NOT have direct EMX2 access — the daemon handles all API communication.

Use wrapper scripts when multi-process orchestration, host-level module systems, or setup that doesn't fit inside a single container exec is needed. Use Apptainer containers when reproducible, isolated execution with a single SIF image is preferred.

5.2 Rationale: Why Hybrid Profiles

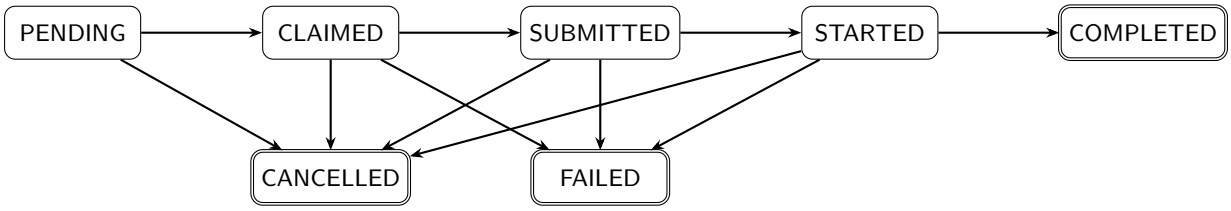
Three models were considered:

1. **Full embedding** — Slurm parameters in EMX2 payloads. Rejected: couples EMX2 to cluster configuration and violates institutional scheduling governance.
2. **Full delegation** — no hint from EMX2 at all. Rejected: EMX2 cannot express workload intent, making it impossible to distinguish a lightweight job from a GPU-heavy one.
3. **Hybrid profiles** (proposed) — EMX2 expresses intent through a logical profile; the HPC side maps it to concrete resources.

The hybrid model keeps scheduling policy within HPC governance while letting EMX2 express meaningful workload requirements. Cluster configuration can change without protocol changes.

6 Job Lifecycle

A job MUST pass through a strict state machine. Every transition is recorded as a sub-resource and the full history is queryable as an audit log.



From	To	Initiated by	Trigger
PENDING	CLAIMED	Head node	Atomic claim
PENDING	CANCELLED	EMX2 or user	Cancel before claim
CLAIMED	SUBMITTED	Head node	After `sbatch`

From	To	Initiated by	Trigger
CLAIMED	FAILED	EMX2 or Head node	Timeout or submission error
CLAIMED	CANCELLED	Head node or EMX2	Cancel before submission
SUBMITTED	STARTED	Daemon (monitoring Slurm state)	Execution begins
SUBMITTED	FAILED	Head node or EMX2	Slurm rejection or timeout
SUBMITTED	CANCELLED	Head node or EMX2	Cancel; head node issues `scancel`
STARTED	COMPLETED	Daemon (monitoring Slurm state)	Outputs committed; `output_artifact_id` set
STARTED	FAILED	Daemon (monitoring Slurm state)	Runtime error, hash mismatch, or timeout
STARTED	CANCELLED	EMX2	Cancel; daemon issues `scancel`

All other transitions MUST be rejected with `409 Conflict`. Jobs in terminal states (COMPLETED, FAILED, CANCELLED) MUST NOT transition further.

Jobs MAY be deleted via `DELETE /api/hpc/jobs/{id}`. Non-terminal jobs MUST be automatically cancelled before deletion. The transition history is deleted with the job.

6.1 Failure Recovery

The protocol is designed to converge to a consistent state after any single failure.

Idempotent transitions. A transition request is considered identical when `job_id`, `status`, `worker_id`, and all payload fields match a previously accepted transition. Duplicates SHOULD return `200 OK`. Non-identical submissions to the same state MUST return `409 Conflict`. This allows safe retries on network failure.

Timeout-driven state progression. Two enforcement tiers are proposed to prevent jobs from stalling indefinitely:

- **Per-job timeout (EMX2-enforced).** Jobs MAY carry an optional `timeout_seconds` field. EMX2 checks CLAIMED and STARTED jobs lazily (on each poll cycle). If `claimed_at + timeout_seconds < now` for a CLAIMED job, or `started_at + timeout_seconds < now` for a STARTED job, EMX2 transitions the job to FAILED with a timeout detail message. This provides fine-grained, per-job control when callers know the expected duration.
- **Per-profile timeout (daemon-enforced).** Each profile in the daemon config would carry `claim_timeout_seconds` (default 300) and `execution_timeout_seconds` (default 0 = rely on Slurm wall time). The daemon checks tracked jobs against these limits on each monitor cycle. On timeout, it transitions the job to FAILED and issues `scancel` if a Slurm job ID is known. This acts as a safety net for jobs that lack a per-job timeout.

Infrastructure termination. If Slurm kills a job unexpectedly (node failure, preemption, wall-time exceeded), the daemon detects this via `squeue`/`sacct` on the next monitor cycle and posts a FAILED transition. The workload (whether container or wrapper script) has no direct EMX2 access — its only output channel is the filesystem: exit code, output files in `HPC_OUTPUT_DIR`, and an optional `.hpc_progress.json` progress file. The daemon is responsible for interpreting these signals and posting appropriate transitions.

Concurrency control. Workers declare `max_concurrent_jobs` during registration and are responsible for not over-claiming. EMX2 MAY optionally enforce an upper bound.

7 Artifact Store

Artifacts are the primary data objects in the proposed system: job inputs, job outputs, model weights, execution logs, container images. This section describes how they would be classified, where they live, how their integrity is ensured, and how their lifecycle is managed.

7.1 Classification

Every artifact is described along two dimensions.

Type is a free-text label describing what the artifact is. No fixed ontology is proposed — users write whatever is meaningful for their context: `csv`, `parquet`, `onnx-model`, `vcf`, `log`, `report`, `sif`, etc. Per-file `content_type` covers media type details, so a single field suffices for artifact-level classification.

Name is a human-readable identifier for the artifact. Names are optional but strongly encouraged — without one, artifacts would be identified only by truncated UUIDs in the UI. The daemon SHOULD auto-generate names like `output-<job-id-prefix>` for job outputs.

Residence specifies where the content physically lives.

Residence	Content URI	Access pattern
`managed`	Artifact API endpoint	Upload/download via API; also S3-compatible endpoint.
`posix`	`file:///nfs/...`	Direct filesystem read from any node with the NFS mount.
`s3`	`s3://bucket/key`	Direct access with presigned URLs or credentials.
`http`	`https://...`	Direct download; supports range requests.
`reference`	N/A	Metadata-only; EMX2 tracks but does not store or proxy.

7.2 Residence: NFS

The cluster's NFS export is mounted on both the head node and all compute nodes. This makes it the natural location for large, frequently-reused artifacts: model weights, pre-built indices, and Apptainer SIF images. Data produced by one job would be immediately available to the next.

The `posix` residence registers artifacts that live on NFS. The content URI is a `file://` path referencing the absolute mount location. The Apptainer runtime reads directly from NFS with no transfer overhead — the fastest access pattern for data already co-located with compute.

Since all nodes share the same NFS export, mount availability is not a per-node concern. Immutability would be enforced by convention: operators MUST ensure that committed paths are not modified or deleted outside the protocol. Hash verification still applies — the runtime checks SHA-256 hashes before use, just as for any other residence.

7.3 Residence: Managed Repository

Managed artifacts would be stored in EMX2's database using the FILE column type. The proposed artifact file API exposes an S3-minimal surface — path-based `PUT` (upload), `GET` (download), `HEAD` (metadata), and `DELETE` operations on individual files within an artifact, plus paginated listing. This maps cleanly to WebDAV semantics and makes future S3-compatible gateway implementation straightforward.

The file API uses path-addressed URLs: `/api/hpc/artifacts/{id}/files/{path}`. Paths are logical names within the artifact (e.g. `data.parquet`, `model/weights.bin`) and support any depth. The server computes SHA-256 on upload and returns it in the response; clients do not need to pre-compute hashes for individual file uploads (though the overall artifact hash is provided at commit time). For browser-based uploads, the client SHOULD send a raw binary PUT body and compute the commit-time SHA-256 via the SubtleCrypto API; no multipart encoding is required.

For analytical tools (DuckDB, pandas), committed artifacts could be accessed via the GET endpoint with standard HTTP range requests. A future S3-compatible gateway could proxy these paths to provide native S3 connector support.

7.4 Multi-File Artifacts and Integrity

Some artifacts consist of multiple files: a model with a tokenizer sidecar, a VCF with a tabix index. Multi-file artifacts MUST include a file manifest listing each file's path, size, and individual SHA-256 hash.

For single-file artifacts, the content hash is the SHA-256 of the file bytes. For multi-file artifacts, the top-level hash is a tree hash: `SHA256(concat(for each file in sorted(paths): path + ":" + sha256_hex(file_bytes)))`. Any modification to any constituent file would be detectable.

Input artifacts MUST be COMMITTED before a job can reference them. The daemon verifies hashes before execution — for managed artifacts it downloads and hashes locally; for NFS artifacts it reads from the mount. A mismatch MUST result in a FAILED transition with reason `input_hash_mismatch`. Output artifacts MUST be immutable after commit.

7.5 Schema Metadata

Tabular artifacts (e.g. `type: "parquet"` or `type: "csv"`) SHOULD include a `schema` field describing column names, types, nullability, row count, and (for Parquet) row group count. This would be extracted automatically from the Parquet file footer at commit time, so consumers can discover data shape without downloading the file.

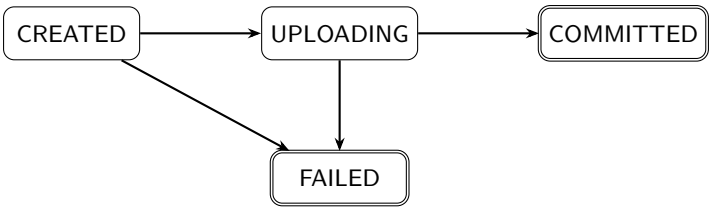
This metadata makes artifacts directly queryable. Tools like DuckDB can read a Parquet file from its NFS path or HTTP URL using range requests — fetching the footer first, then only the needed columns and rows. For NFS-resident artifacts this happens with zero network overhead. In practice, EMX2 application code or analytical scripts could use this to inspect job outputs without pulling entire datasets: a SQL query against the artifact's `content_url` (or NFS path) would return results in place.

7.6 Execution Logs

The daemon SHOULD upload execution logs as artifacts of type `log`, governed by the same retention policy and integrity model as other artifacts. Log artifacts would be referenced alongside outputs in the COMPLETED (or FAILED) transition. Structured JSONL is recommended over plain text for machine queryability.

7.7 Artifact Lifecycle

Managed artifacts would pass through a state machine:



External artifacts (POSIX, S3, HTTP, reference) skip the upload phase: REGISTERED → COMMITTED or REGISTERED → FAILED.

Artifacts MUST be immutable after COMMITTED. If an artifact stalls in CREATED or UPLOADING with no activity within a configured timeout, it SHOULD transition to FAILED and become eligible for garbage collection.

7.8 Job→Artifact Link

Jobs reference output artifacts via the `output_artifact_id` field, which is a foreign key to the `HpcArtifacts` table. When the daemon completes a job and uploads (or registers) output artifacts, it passes the `output_artifact_id` in the COMPLETED transition request. EMX2 stores this link on the job record, making it queryable via GraphQL (`output_artifact_id { id name type status { name } }`).

Input artifacts are referenced in the job's `inputs` field (a JSON array of artifact IDs). The daemon stages input artifacts before execution: for managed artifacts it downloads files via GET; for posix artifacts it symlinks the `file://` path into the job's input directory. The output residence for each profile is configured in the daemon config via an `artifact_residence` field on each profile entry. This two-residence model means that large datasets on NFS incur zero transfer overhead, while smaller browser-uploaded artifacts are served from the managed store.

8 API Design

This section describes the principles governing the proposed API. Full endpoint specifications with request and response payloads are in Appendix A.

8.1 Versioning

The API SHOULD be versioned via the `X-EMX2-API-Version` request header rather than a URL path prefix. Versions are date-based strings (e.g. `2025-01`). This keeps URLs stable across versions and avoids cascading changes to hypermedia links. Missing header → `400 Bad Request`; unsupported version → `400 Bad Request`.

8.2 Request Headers and Traceability

Every request from a worker or runtime MUST include a standard set of headers:

Header	Required	Purpose
`X-EMX2-API-Version`	Yes	Protocol version (date-based, e.g. `2025-01`).
`X-Request-Id`	Yes	Unique per-request identifier (UUID v4).
`X-Timestamp`	Yes	Request creation time; used for HMAC verification and replay prevention.
`X-Nonce`	When HMAC enabled	Cryptographically random single-use value; replay prevention.
`X-Trace-Id`	No	Identifier spanning a logical operation, e.g. an entire job lifecycle.
`X-Worker-Id`	No	Worker identifier; used by some endpoints (e.g. cancel).
`Authorization`	When HMAC enabled	`HMAC-SHA256 <hex-signature>` (see Authentication and Trust).

EMX2 MUST echo `X-Request-Id` in error responses for traceability.

8.3 Resource Model and Hypermedia

The API is organized around two resources: **jobs** and **artifacts**. State transitions on jobs are a **transitions** sub-resource: each transition is a created resource (`POST` returns `201 Created`), the history is queryable, and the job representation includes `_links` advertising legal next actions. Clients follow links rather than hard-coding URL patterns (HATEOAS). All URLs in `_links` fields MUST be treated as opaque — clients dereference them as-is.

8.4 Error Responses

Client errors MUST return structured JSON with `type`, `title`, `status`, and `detail` fields, following the RFC 9457 (Problem Details for HTTP APIs) structure. Whether to formally adopt the `application/problem+json` media type is an open deployment decision.

8.5 Endpoint Summary

All endpoints are proposed under `/api/hpc`. Detailed specifications are in Appendix A.

Workers API

Method	Path	Purpose
`POST`	`/workers/register`	Register or update a worker and its capabilities
`POST`	`/workers/{id}/heartbeat`	Lightweight keepalive
`DELETE`	`/workers/{id}`	Remove a stale worker

Jobs API

Method	Path	Purpose
POST	/jobs	Create a new job (pending)
GET	/jobs	List/filter jobs (paginated)
GET	/jobs/{id}	Retrieve a single job
POST	/jobs/{id}/claim	Atomically claim a pending job
POST	/jobs/{id}/transition	Report a state transition
POST	/jobs/{id}/cancel	Cancel from any non-terminal state
DELETE	/jobs/{id}	Delete a job and its history
GET	/jobs/{id}/transitions	Ordered transition audit log

Artifact API

Method	Path	Purpose
POST	/artifacts	Create an artifact (managed or external)
GET	/artifacts/{id}	Retrieve artifact metadata
PUT	/artifacts/{id}/files/{path}	Upload a file by path
GET	/artifacts/{id}/files/{path}	Download a file
HEAD	/artifacts/{id}/files/{path}	File metadata (existence, hash, size)
DELETE	/artifacts/{id}/files/{path}	Delete a file (before commit only)
GET	/artifacts/{id}/files	List files (paginated, prefix-filterable)
POST	/artifacts/{id}/commit	Commit with top-level SHA-256
POST	/artifacts/{id}/files	Upload (legacy multipart; prefer PUT)

Health

Method	Path	Purpose
GET	/health	Liveness check (exempt from authentication)

9 Authentication and Trust

The protocol operates across a trust boundary between EMX2 (public internet or institutional network) and the HPC environment (internal cluster network). Every API call crosses this boundary, so the security model must answer three questions: who is making this request, has the request been tampered with, and is this request fresh (not a replay of an earlier one)?

9.1 Proposed Authentication Mechanism

Every request from the HPC side to EMX2 MUST carry a set of standard headers that together form an authentication envelope:

```
X-EMX2-API-Version: 2025-01
X-Request-Id:       <UUID v4>
X-Timestamp:        <unix epoch seconds>
X-Nonce:            <random value, used exactly once>
Authorization:      HMAC-SHA256 <hex-encoded signature>
```

The `Authorization` header contains an HMAC-SHA256 signature computed over a canonical request string: `METHOD\nPATH\nSHA256(body)\nTIMESTAMP\nNONCE`. This ensures:

- **Origin** — EMX2 can verify which worker sent the request, because only that worker has the secret needed to produce a valid signature.
- **Integrity** — if any part of the request (body, path, headers) is altered in transit, the signature will not match and EMX2 MUST reject it.
- **Freshness** — the `X-Timestamp` tells EMX2 when the request was created, and the `X-Nonce` is a random value that MUST NOT be reused. EMX2 MUST reject requests whose timestamp is too far in the past (e.g. more than 5 minutes) and MUST reject any nonce it has seen before. Together these prevent an attacker from capturing a valid request and re-submitting it later.

9.2 Provisioning

Each head node MUST be provisioned with a unique **`worker_id`** that identifies the head node across all API calls, and credentials for at least one of the supported authentication mechanisms (see below).

These credentials are configured in EMX2. Revoked or changed credentials take effect immediately.

9.3 Supported Authentication Mechanisms

Every daemon-to-EMX2 request MUST be authenticated by at least one of the following mechanisms. Deployments COULD use either; HMAC-SHA256 is preferred for production.

Mechanism	How it works	Notes
HMAC-SHA256 *(preferred)*	Worker and EMX2 share a secret key. The worker computes a keyed hash over a canonical request string; EMX2 recomputes it and compares. Transmitted as `Authorization: HMAC-SHA256 <hex>`.	Provides per-request integrity, origin verification, and replay protection. The shared secret SHOULD be stored in a file with restricted permissions (mode `0600`) and referenced via `shared_secret_file` in the daemon configuration.
JWT / API token	Worker authenticates with an EMX2 API token via the `x-molgenis-token` header. EMX2 validates the token through its standard token verification.	Simpler to set up; useful for development or when the infrastructure already has token management. Does not provide per-request integrity or replay protection.

The shared secret for HMAC SHOULD be stored as a database setting (`MOLGENIS_HPC_SHARED_SECRET`, minimum 32 characters). When no secret is configured, HMAC verification is disabled (suitable for development only).

When HMAC is enabled, replay protection SHOULD enforce a 5-minute timestamp drift window and an LRU nonce cache.

9.4 Server-Side Authentication Cascade

The `/api/hpc/*` before-handler accepts three authentication methods, tried in order:

1. **HMAC-SHA256** — daemon requests carrying an `Authorization: HMAC-SHA256 <signature>` header. The server recomputes the signature over the canonical request string (including query parameters) using the shared secret and compares.
2. **JWT token** — requests with an `x-molgenis-token` header. The server validates the token via EMX2's standard JWT verification (`JWTgenerator`).
3. **Session cookie** — browser requests from signed-in EMX2 users. The server reads the `username` attribute from the servlet session (set by the standard EMX2 sign-in flow).

If none of the three methods yields an authenticated identity, the server returns `401 Unauthorized`. The health endpoint (`/api/hpc/health`) is exempt from authentication.

This cascade allows the HPC daemon to authenticate via HMAC (the primary path), while the browser-based management UI authenticates via the user's existing EMX2 session without needing access to the shared secret.

9.5 What EMX2 Enforces

EMX2 is the sole authority for job state, lifecycle transitions, and artifact metadata. Workers MUST NOT unilaterally change anything — they can only *request* transitions, which EMX2 validates against the state machine before accepting. This means even a compromised worker can only submit requests that are legal given the current state; it cannot, for example, mark someone else's job as completed or overwrite a committed artifact.

10 Summary, Trade-offs, and Open Questions

10.1 What This Proposal Provides

A minimal, deterministic bridge between EMX2 and HPC infrastructure with these invariants:

- **Outbound-only communication.** EMX2 never initiates connections to the cluster.
- **Flexible execution.** Either Apptainer containers (SIF images on NFS) or wrapper scripts, invoked by Slurm on compute nodes.
- **NFS as the primary shared data path.** Artifacts co-located with compute require no transfer.
- **Resource-oriented API with HATEOAS.** Clients discover actions from server responses.
- **Typed, content-addressed artifacts.** A single metadata model governs everything from queryable Parquet tables to multi-gigabyte model weights, with SHA-256 integrity verification.
- **Idempotent transitions and timeout-based recovery.** The system converges after any single failure.

10.2 Key Trade-offs

Polling vs. push. The outbound-only constraint requires the head node to poll EMX2 for new jobs, introducing latency proportional to the poll interval. A shorter interval reduces latency but increases API load. For the expected workload (long-running GPU jobs), 10–30 seconds is likely acceptable, but this should be validated under realistic load.

Hybrid profiles. EMX2 expresses workload intent; the HPC side interprets it. This preserves scheduling governance but means EMX2 cannot guarantee exact resource allocation. The head node's profile-to-Slurm mapping is an out-of-band dependency that must be kept in sync manually.

NFS immutability by convention. The protocol registers NFS paths as artifacts but cannot enforce immutability on them. If an operator modifies a file after it has been committed, the hash check will catch it at runtime — but the job will fail rather than being prevented. In environments with strict data governance this may need filesystem-level write protection (e.g. read-only snapshots or chattr).

S3-minimal file surface. The proposed artifact file API exposes path-based GET/PUT/HEAD/DELETE operations that map to S3 semantics (`GetObject`, `PutObject`, `HeadObject`, `DeleteObject`). This is sufficient for the initial use case and makes a future S3-compatible gateway straightforward to implement. Until then, analytical tools would access managed artifacts via HTTP GET with range request support.

Authentication mechanism. Two mechanisms are supported: HMAC-SHA256 (recommended for production, provides per-request integrity and replay protection) and JWT/API tokens. Browser-based access is handled via session cookies. See §8 for details.

10.3 Open Design Decisions

Decision	Options	Considerations
Artifact retention	TTL, reference-counted, or manual	Out of protocol scope, but the store must accommodate the chosen strategy.
S3-compatible gateway	MinIO proxy, custom gateway, or none	The proposed path-based API maps to S3 semantics; a gateway would add DuckDB/pandas native S3 support.

Appendix A: API Reference

Full endpoint specifications. All endpoints require authentication as described in §8. URLs shown here are illustrative; in practice, clients MUST follow `_links` from server responses.

A.1 Workers API

POST /api/hpc/workers/register

Registers a worker or updates its registration. Idempotent — subsequent calls update the heartbeat timestamp and replace the capability set.

```
{
  "worker_id": "hpc-headnode-01",
  "hostname": "login-node.cluster.local",
  "capabilities": [
    {
      "processor": "text-embedding:v3",
      "profile": "gpu-medium",
      "max_concurrent_jobs": 4
    }
  ]
}
```

Response: `200 OK` with worker metadata and HATEOAS links.

```
{
  "worker_id": "hpc-headnode-01",
  "hostname": "login-node.cluster.local",
  "registered_at": "2026-02-21T10:00:00",
  "last_heartbeat_at": "2026-02-21T10:00:00",
  "_links": {
    "self": { "href": "/api/hpc/workers/hpc-headnode-01", "method": "GET" },
    "heartbeat": { "href": "/api/hpc/workers/register", "method": "POST" },
    "jobs": { "href": "/api/hpc/jobs?status=PENDING", "method": "GET" }
  }
}
```

POST /api/hpc/workers/{id}/heartbeat

Lightweight heartbeat. Updates `last_heartbeat_at` without re-submitting capabilities. The daemon SHOULD send this periodically (default: every 120 seconds) between poll cycles.

Response: `200 OK` with `{"worker_id": "...", "status": "ok"}`.

DELETE /api/hpc/workers/{id}

Removes a worker and its capabilities. Jobs previously assigned to this worker retain their history but have their `worker_id` nullified. Useful for cleaning up stale workers that are no longer active.

Response: `204 No Content`, `404 Not Found`.

A.2 Jobs API

POST /api/hpc/jobs

Creates a new job in PENDING status.

```
{
  "processor": "text-embedding:v3",
  "profile": "gpu-medium",
  "submit_user": "researcher@example.org",
  "parameters": { "model": "multilingual-e5-large", "batch_size": 256 },
  "inputs": { "dataset": "corpus-01" }
}
```

Response: `201 Created`

```
{
  "id": "550e8400-e29b-41d4-a716-446655440000",
  "status": "PENDING",
  "_links": {
    "self": { "href": "/api/hpc/jobs/550e8400-...", "method": "GET" },
    "claim": { "href": "/api/hpc/jobs/550e8400-.../claim", "method": "POST" },
    "cancel": { "href": "/api/hpc/jobs/550e8400-.../cancel", "method": "POST" }
  }
}
```

GET /api/hpc/jobs

Lists jobs with optional filtering and pagination. Query parameters: `status`, `processor`, `profile`, `limit` (default 100), `offset` (default 0). When status is omitted, the default SHOULD be `PENDING` (optimized for worker polling).

Response: `200 OK` with paginated result.

```
{
  "items": [ { "id": "...", "status": "PENDING", "processor": "text-embedding:v3", ... } ],
  "count": 2,
  "total_count": 42,
  "limit": 100,
  "offset": 0,
  "_links": { "self": { "href": "/api/hpc/jobs", "method": "GET" } }
}
```

POST /api/hpc/jobs/{id}/claim

Atomically claims a job. Returns `409 Conflict` if already claimed, `404` if not found.

Request: `{ "worker_id": "hpc-headnode-01" }`

Response: `200 OK` with the job in CLAIMED state, including `_links` for `submit` and `cancel`.

```
{
  "id": "550e8400-...",
```

```
  "status": "CLAIMED",
  "worker_id": "hpc-headnode-01",
  "processor": "text-embedding:v3",
  "profile": "gpu-medium",
  "_links": {
    "self": { "href": "/api/hpc/jobs/550e8400-...", "method": "GET" },
    "transitions": { "href": "/api/hpc/jobs/550e8400-.../transitions", "method": "GET" },
    "submit": { "href": "/api/hpc/jobs/550e8400-.../transition", "method": "POST" },
    "cancel": { "href": "/api/hpc/jobs/550e8400-.../cancel", "method": "POST" }
  }
}
```

POST /api/hpc/jobs/{id}/transition

Reports a state transition. MUST reject invalid transitions with `409 Conflict`. Idempotent: re-posting an identical transition returns `200 OK`. Response includes the updated job.

SUBMITTED (head node, after `sbatch`):

```
{ "status": "SUBMITTED", "worker_id": "hpc-headnode-01", "detail": "sbatch id 45678", "slurm_job_id": "45678" }
```

STARTED (daemon monitor):

```
{ "status": "STARTED", "worker_id": "hpc-headnode-01", "detail": "running on node-05" }
```

COMPLETED (after outputs committed):

```
{
  "status": "COMPLETED",
  "worker_id": "hpc-headnode-01",
  "detail": "exit code 0",
  "output_artifact_id": "art_abc123-..."
}
```

FAILED (head node or daemon):

```
{ "status": "FAILED", "worker_id": "hpc-headnode-01", "detail": "input_hash_mismatch" }
```

POST /api/hpc/jobs/{id}/cancel

Convenience endpoint for cancellation. Transitions the job to CANCELLED from any non-terminal state. The head node SHOULD issue `scancel` if a Slurm job ID is known.

Response: `200 OK` with updated job, `409 Conflict` if already terminal.

DELETE /api/hpc/jobs/{id}

Deletes a job and its transition history. Non-terminal jobs MUST be automatically cancelled before deletion.

Response: `204 No Content`, `404 Not Found`.

GET /api/hpc/jobs/{id}/transitions

Ordered transition history (audit log).


```
{
  "items": [
    { "id": "tr_001", "from_status": null, "to_status": "PENDING",
      "timestamp": "2026-02-21T10:28:00", "worker_id": null, "detail": "Job created" },
    { "id": "tr_002", "from_status": "PENDING", "to_status": "CLAIMED",
      "timestamp": "2026-02-21T10:29:00", "worker_id": "hpc-headnode-01", "detail": "Claimed by worker hpc-headnode-
  ],
  "count": 2
}
```


Error response example

Follows RFC 9457 (Problem Details for HTTP APIs) structure.


```
{
  "title": "Conflict",
  "status": 409,
  "detail": "Cannot transition job 550e8400-... from PENDING to STARTED"
}
```


A.3 Artifact API

POST /api/hpc/artifacts

Creates an artifact. Managed artifacts start in CREATED; external artifacts (posix, s3, http, reference) start in REGISTERED.

Managed: `{ "name": "my-dataset", "type": "parquet", "residence": "managed" }`

NFS: `{ "name": "output-abc123", "type": "blob", "residence": "posix", "content_url": "file:///nfs/outputs/job-123" }`

S3: `{ "name": "analysis-results", "type": "parquet", "residence": "s3", "content_url": "s3://..." }`

Response: `201 Created`


```
{
  "id": "art_abc123-...",
  "name": "my-dataset",
  "type": "parquet",
  "status": "CREATED",
  "_links": {
    "self": { "href": "/api/hpc/artifacts/art_abc123-...", "method": "GET" },
    "upload": { "href": "/api/hpc/artifacts/art_abc123-.../files/{path}", "method": "PUT" },
    "upload_legacy": { "href": "/api/hpc/artifacts/art_abc123-.../files", "method": "POST" },
    "files": { "href": "/api/hpc/artifacts/art_abc123-.../files", "method": "GET" }
  }
}
```

GET /api/hpc/artifacts/{id}

Returns full metadata with HATEOAS links. Links vary by status: CREATED/UPLOADING include `upload` and (for UPLOADING) `commit`; COMMITTED includes `download`; all include `files`.

Managed artifact (committed):

```
{
  "id": "art_abc",
  "name": "my-dataset", "type": "parquet", "residence": "managed",
  "status": "COMMITTED", "sha256": "b3a3f0...", "size_bytes": 52428800,
  "content_url": null,
  "created_at": "2026-02-21T10:00:00", "committed_at": "2026-02-21T10:05:00",
  "_links": {
    "self": { "href": "/api/hpc/artifacts/art_abc", "method": "GET" },
    "download": { "href": "/api/hpc/artifacts/art_abc/files/{path}", "method": "GET" },
    "files": { "href": "/api/hpc/artifacts/art_abc/files", "method": "GET" }
  }
}
```

NFS artifact: `"residence": "posix", "content_url": "file:///nfs/data/outputs/embeddings.parquet"`

S3 artifact: `"residence": "s3", "content_url": "s3://data-lake/outputs/analysis.parquet"`

PUT /api/hpc/artifacts/{id}/files/{path}

Uploads a file to an artifact by path. The `{path}` segment is the logical file name within the artifact (e.g. `data.parquet`, `model/weights.bin`). Upserts: if a file already exists at that path, it is replaced. Transitions the artifact from CREATED to UPLOADING on the first upload.

Accepts two body formats:

- **Raw binary** (preferred): `Content-Type` describes the file's media type; body is the raw file bytes. The server computes SHA-256 and stores the file.
- **Multipart**: `Content-Type: multipart/form-data` with a `file` part and optional `content_type` form param.

Request (raw binary):

```
PUT /api/hpc/artifacts/art_abc/files/data.parquet
Content-Type: application/vnd.apache.parquet
X-EMX2-API-Version: 2025-01
...

<raw file bytes>
```

Response: `201 Created`

```
{
  "id": "file-uuid-...",
  "artifact_id": "art_abc",
  "path": "data.parquet",
  "sha256": "b3a3f0...",
```

```
  "size_bytes": 52428800
}
```

HMAC note: For non-JSON request bodies (raw binary uploads), the HMAC signature MUST be computed over an empty string rather than the file bytes. This avoids encoding issues with large binary payloads and matches the token auth path.

GET /api/hpc/artifacts/{id}/files/{path}

Downloads file content. Returns the raw bytes with appropriate `Content-Type`, `Content-Disposition: attachment`, `Content-Length`, and `X-Content-SHA256` headers.

For managed artifacts with stored content, serves bytes directly. For posix/external artifacts where the file metadata exists but no binary is stored, returns `302 Found` redirecting to `{content_url}/{path}`.

Response headers:

```
Content-Type: application/vnd.apache.parquet
Content-Disposition: attachment; filename="data.parquet"
Content-Length: 52428800
X-Content-SHA256: b3a3f0...
```

HEAD /api/hpc/artifacts/{id}/files/{path}

Returns file metadata as headers without body content. Useful for checking existence and integrity without downloading.

Response headers: `X-Content-SHA256`, `Content-Length`, `Content-Type`. Status `200 OK` if found, `404 Not Found` otherwise.

DELETE /api/hpc/artifacts/{id}/files/{path}

Deletes a file from an artifact. Only allowed when the artifact is not yet COMMITTED.

Response: `204 No Content` on success, `409 Conflict` if artifact is committed, `404 Not Found` if file does not exist.

GET /api/hpc/artifacts/{id}/files

Lists files in an artifact with pagination and optional prefix filtering.

Query parameters: `prefix` (filter paths starting with this string), `limit` (default 100), `offset` (default 0).

Response: `200 OK`

```
{
  "items": [
    {
      "id": "file-uuid-...",
      "path": "data.parquet",
      "sha256": "b3a3f0...",
      "size_bytes": 52428800,
      "content_type": "application/vnd.apache.parquet",
```

```
      "_links": {
        "content": {
          "href": "/api/hpc/artifacts/art_abc/files/data.parquet",
          "method": "GET"
        }
      }
    }
  ],
  "count": 1,
  "total_count": 1,
  "limit": 100,
  "offset": 0
}
```

POST /api/hpc/artifacts/{id}/files (legacy)

Uploads a file to an artifact. Provided for compatibility with existing clients. Accepts either JSON metadata-only (`{ "path": "...", "sha256": "...", "size_bytes": ... }`) or multipart with a `file` part and optional `content_type` form param. New clients SHOULD prefer `PUT /files/{path}`.

POST /api/hpc/artifacts/{id}/commit

Commits the artifact with a top-level SHA-256 hash and total size. The artifact MUST be in UPLOADING (managed) or REGISTERED (external) status. Immutable after commit — subsequent uploads and deletes MUST be rejected.

Request: `{ "sha256": "abc123...", "size_bytes": 1024 }`

Response: `200 OK` with full artifact metadata.

Artifact examples by residence

Multi-file model on NFS (posix):

```
{
  "id": "art_model_nfs",
  "name": "llama-3-8b", "type": "gguf", "residence": "posix",
  "status": "COMMITTED", "sha256": "d1e2f3...",
  "content_url": "file:///nfs/models/llama-3-8b/"
}
```

File listing for this artifact:

```
{
  "items": [
    { "path": "model.gguf", "size_bytes": 4294967296, "sha256": "a1b2c3..." },
    { "path": "tokenizer.json", "size_bytes": 524288, "sha256": "d4e5f6..." }
  ]
}
```

For posix artifacts, the daemon registers file metadata without binary content. Consumers access files directly via the NFS mount at the `content_url` path. The GET file endpoint returns a `302` redirect to `{content_url}/{path}` for files without stored binary content.

Appendix B: Sequence Diagram