Qorchestration-CERN Codebase Overview

Modular quantum workflow orchestration with Streamlit, Kubernetes and Argo Workflows

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Journal club
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Presentation goal

Explain the concrete logic of the current `qorchestration-v0.2` codebase: how tasks are defined, submitted, executed, archived, and analyzed for Circuit Cutting and SQD workflows.

Executive summary

- **Purpose:** one user-facing console for launching quantum workflows on a Kubernetes cluster.
- **Two first-class modules:** Circuit Cutting and Sample-based Quantum Diagonalization (SQD).
- **Shared core:** cluster validation, Argo submission, runtime handling, artifact archival, QPU secret setup.
- **Execution model:** Streamlit task builder $\rightarrow$ Argo Workflow $\rightarrow$ CPU/GPU/QPU pods $\rightarrow$ PVC artifacts $\rightarrow$ local archive/analysis.

What the codebase demonstrates

- Modular integration, not a monolithic script.
- Backend-aware workflow specifications.
- Reusable launch/archive/analyze path.
- Early validation tests for structure and task generation.

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Why orchestration is needed

Quantum workflow experiments are not a single Python call. They require:

- parameterized task generation;
- backend-specific execution environments;
- repeatable cluster submission;
- shared storage for intermediate artifacts;
- logs, summaries and experiment provenance;
- a UI that hides operational complexity from the user.

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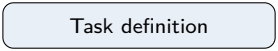

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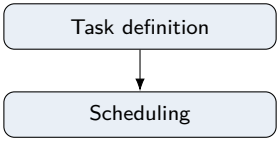

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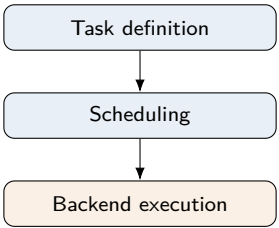

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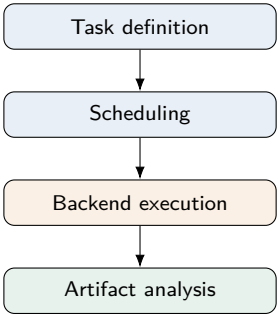

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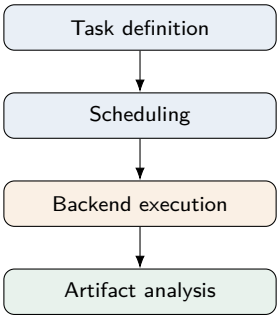

Top-level architecture

Streamlit UI `qorch_integrated/ui/app.py` pages: Cluster setup, QPU setup, SQD, Circuit cutting

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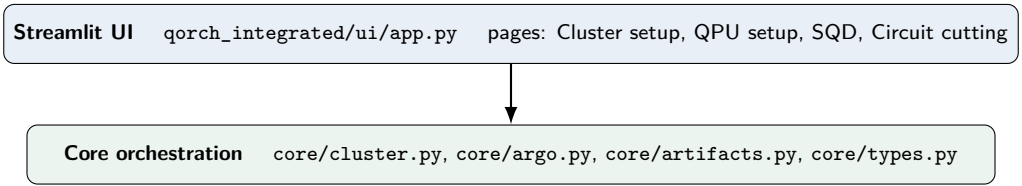

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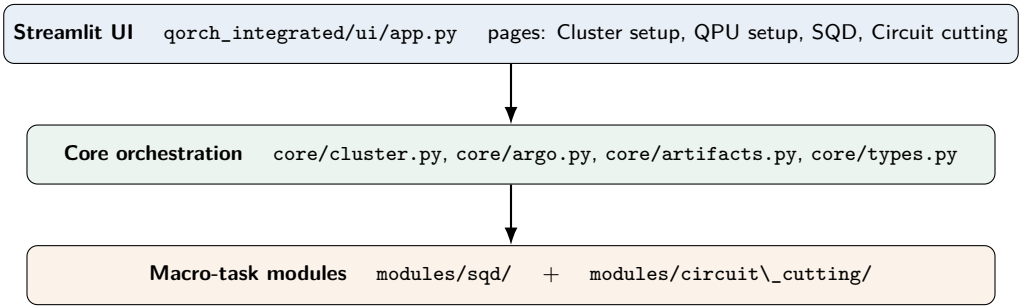

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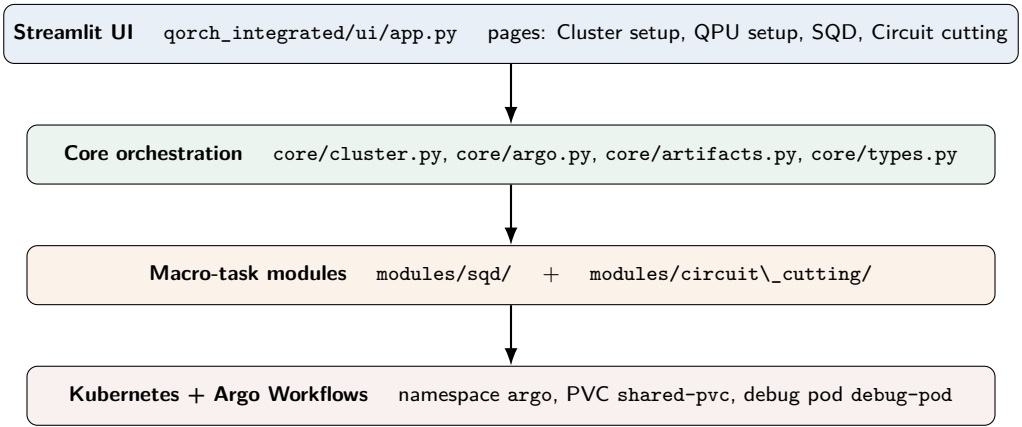

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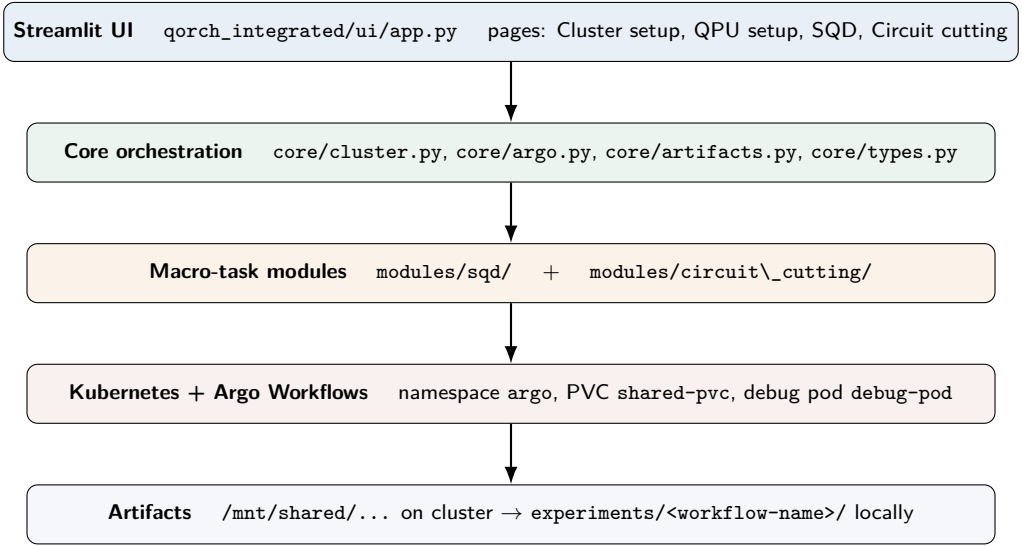

Codebase organization: separation of concerns

Where users enter

`qorch_integrated/ui/app.py`

Streamlit collects configuration and delegates execution to registered modules.

Shared infrastructure

```
core/types.py        # module contract
core/cluster.py      # kubeconfig + checks
core/argo.py         # kubectl wrapper
core/artifacts.py    # archive/log copy
core/qpu.py          # QPU secret setup
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Scientific macro-task modules

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modules/registry.py
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Design rule

Modules own task schemas, workflow YAMLs, Docker assets, executors and analysis. The core layer sees only `MacroTaskModule` and `WorkflowSpec`.

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Module contract: the plug-in mechanism

1. Registry
`modules/registry.py`

UI-facing methods

`render_task_form()` `launch()`
`latest()` `status_line()`

WorkflowSpec declares

Workflow file, launcher script, remote task path, artifact roots and workflow-name prefix.

Reason for the contract

Adding a macro-task should not require rewriting `app.py`; it only needs to respect the interface.

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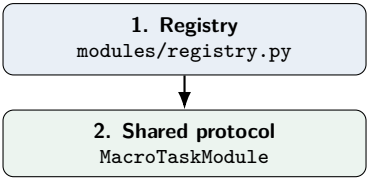

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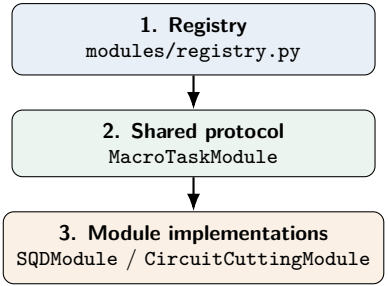

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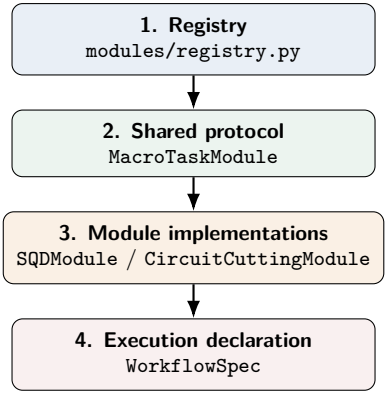

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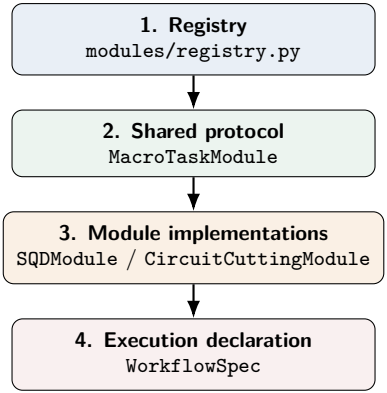

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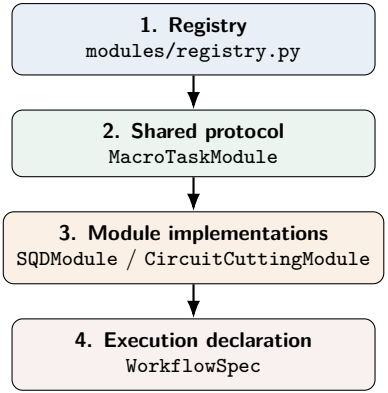

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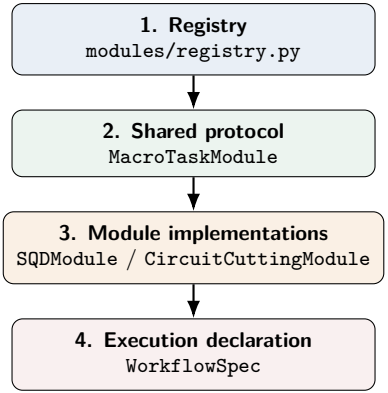

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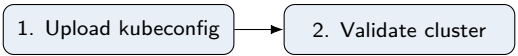
User-facing Streamlit flow

1. Upload kubeconfig

Specific current behavior

`app.py` saves uploaded kubeconfig files under `.runtime/kubeconfigs/`, activates `KUBECONFIG` in-process, validates Argo/PVC/debug-pod access, and provides Back/Next navigation plus a Quit button.

User-facing Streamlit flow



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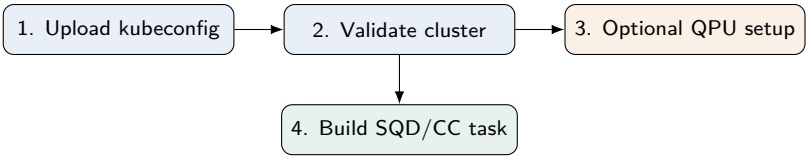

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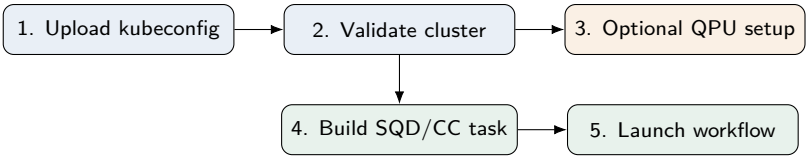

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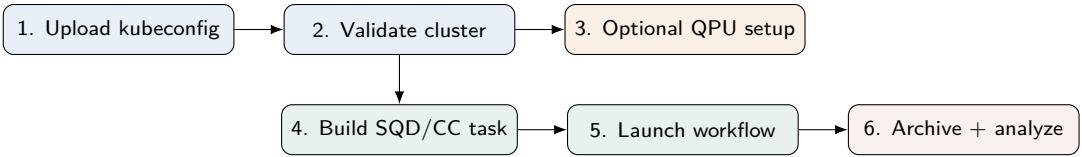

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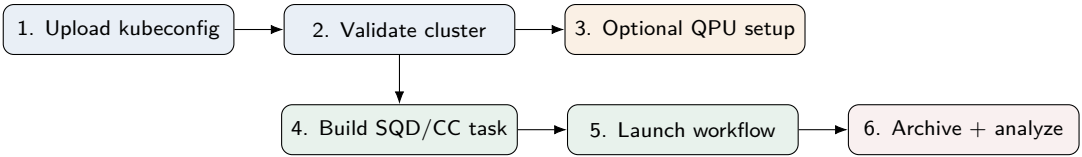

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Core execution path: control flow and data flow

Local task file
`tasks/*.yaml/json`

- `ArgoClient` wraps `kubectl`, discovers latest workflow names, optionally waits for terminal phases, and formats status lines.
- `archive_workflow()` stores workflow YAML, pods table/JSON, pod logs, task copy and copied `/mnt/shared` artifacts.

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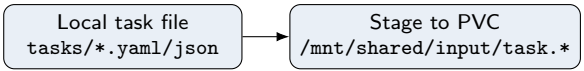

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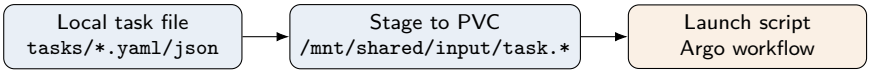

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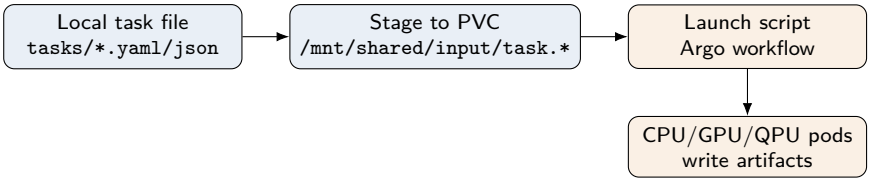

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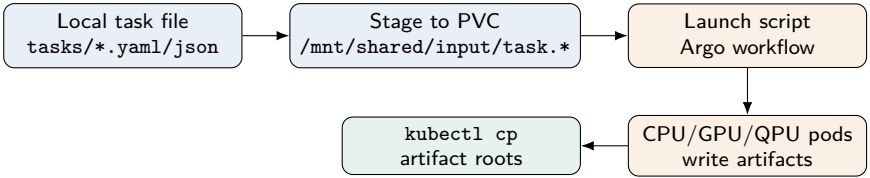

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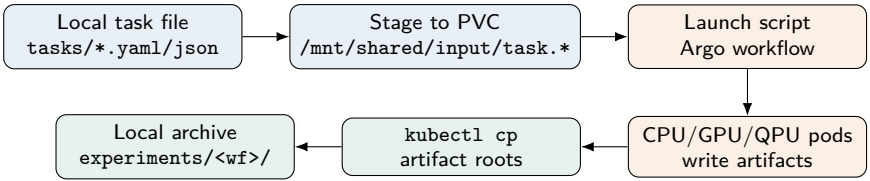

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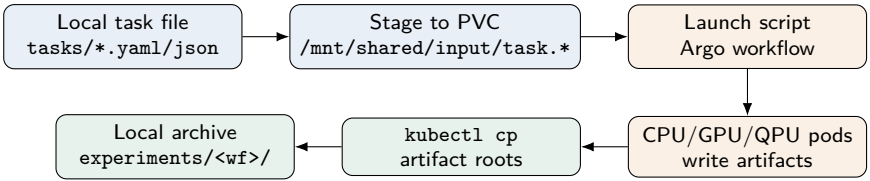

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- `archive_workflow()` stores workflow YAML, pods table/JSON, pod logs, task copy and copied `/mnt/shared` artifacts.

Circuit Cutting module: from a circuit to reconstructed results

Task JSON
circuit, cuts, routing

Key idea

Circuit cutting is a **fan-out/fan-in workflow**: one preparation step creates many subcircuit execution units; reconstruction joins the branch results.

Main files to point at

`task_model.py`, `task_builder.py`, `k8s/argo-workflow.yaml`, `create_subcircuits.py`, `execute_subcircuits_*.py`, `reconstruct.py`, `summarize_workflow.py`.

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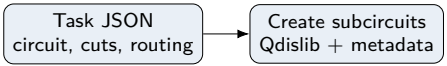

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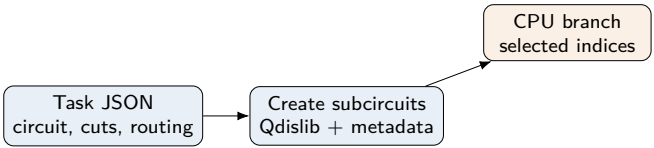

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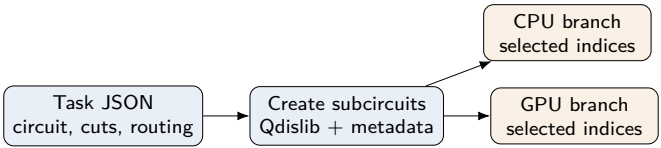

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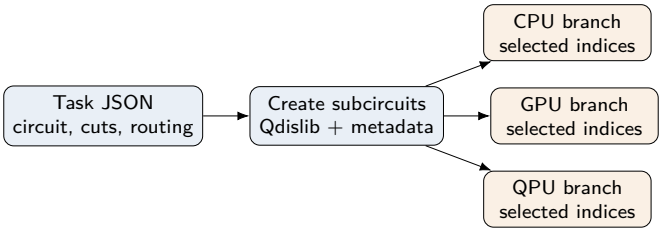

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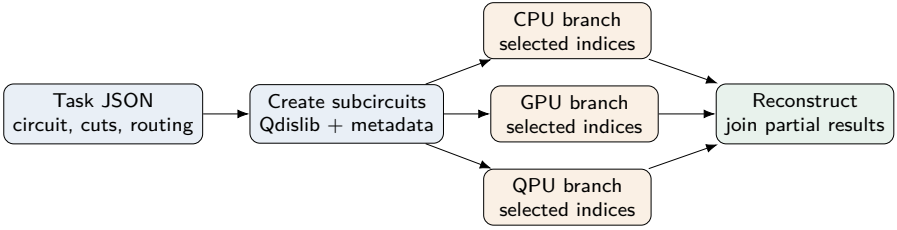

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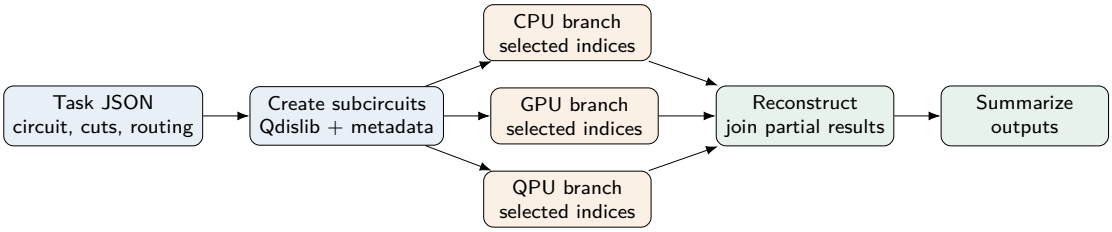

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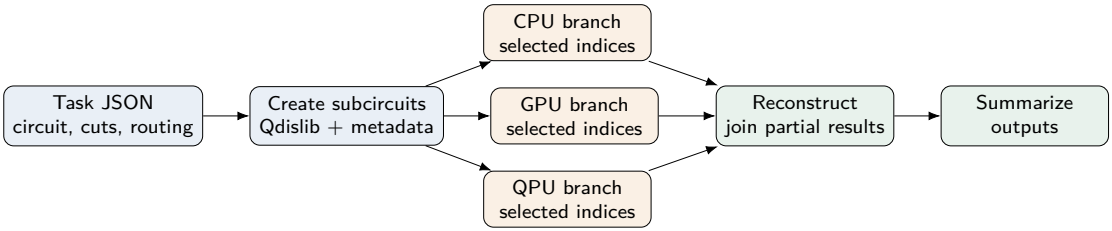

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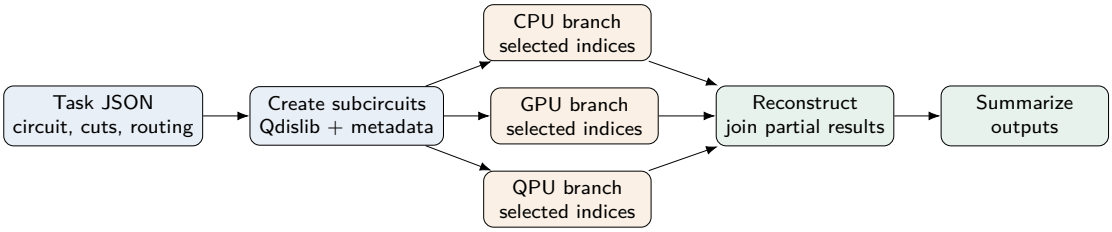

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- Supported circuit families: `ring`, `chain`, `star`, hardware-efficient variants.
- Gate layers include `ry_rz`, `h_ry_rz`, `rx_ry_rz`; entanglers include `cz` and `cx`.
- Cut strategies: explicit, first/last k, evenly spaced, random.
- Routing modes include CPU-only, GPU-only, hybrid, custom, forced CPU/GPU split and automatic.

Automatic execution logic

`CircuitCuttingTaskConfig.validate()` enforces automatic execution only with automatic routing. Smoke tests check that the generated policy matches downstream execution.

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SQD module: workflow logic

Hamiltonian source
manual / IBM N2 / catalog

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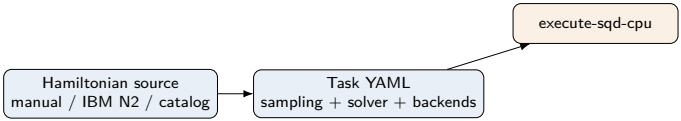

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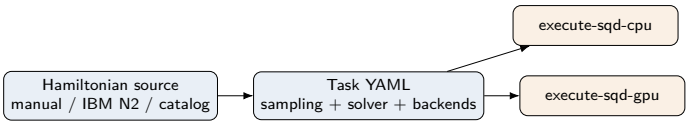

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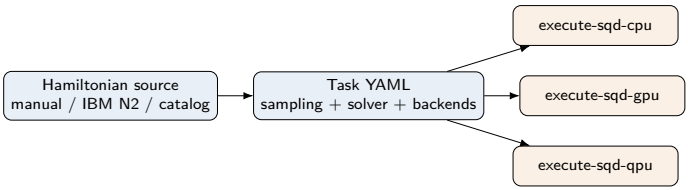

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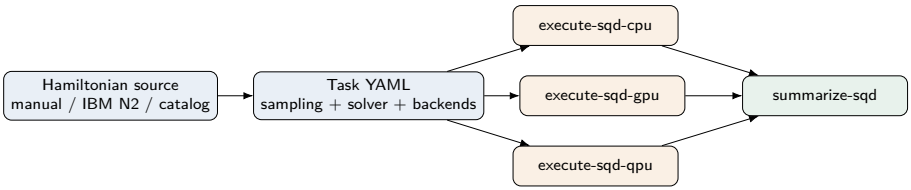

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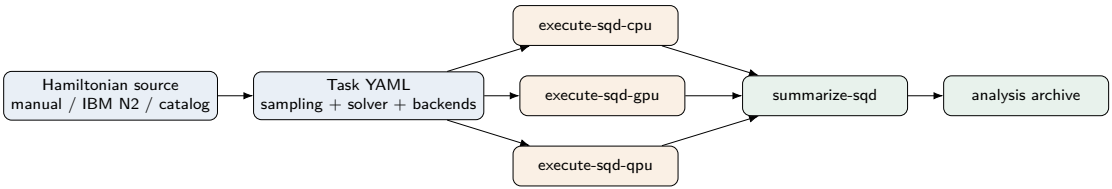

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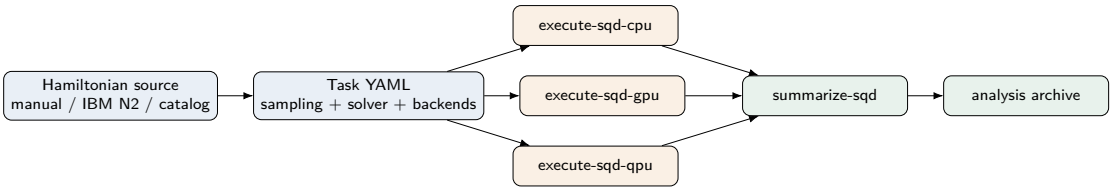

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- **Manual Pauli source:** user writes Pauli terms directly.
- **IBM N2 reference:** built-in reference task support through `build_ibm_n2_task()`.
- **Molecule catalog:** catalog-driven task generation through molecule fixture IDs.
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Current benchmark assets

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- examples: `h2_sto3g.yaml`, `h2o_small_active_space.yaml`, `ibm_n2_reference.yaml`

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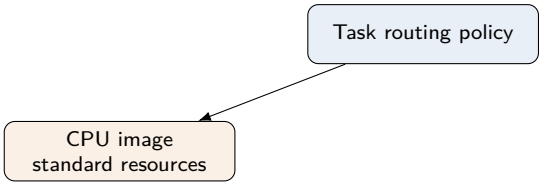

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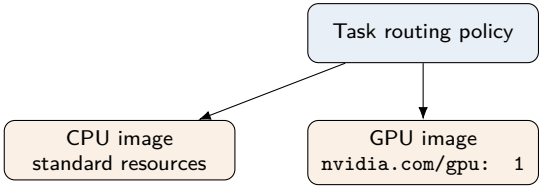

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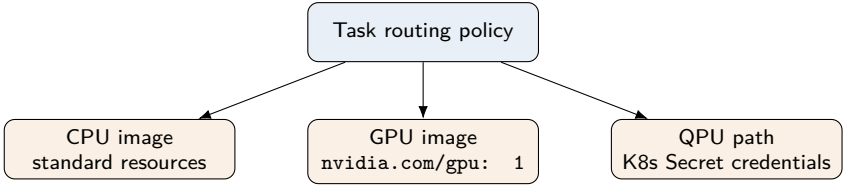

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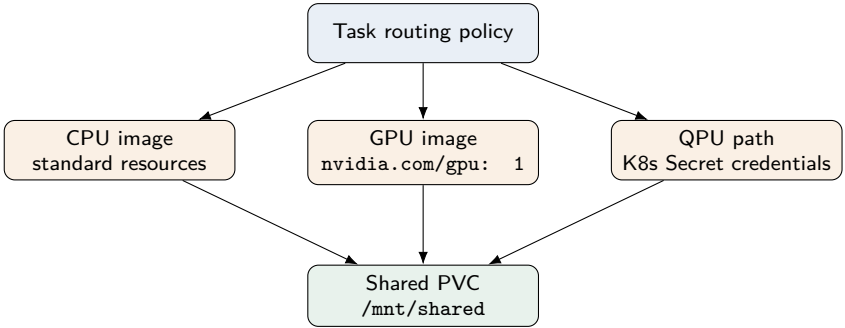

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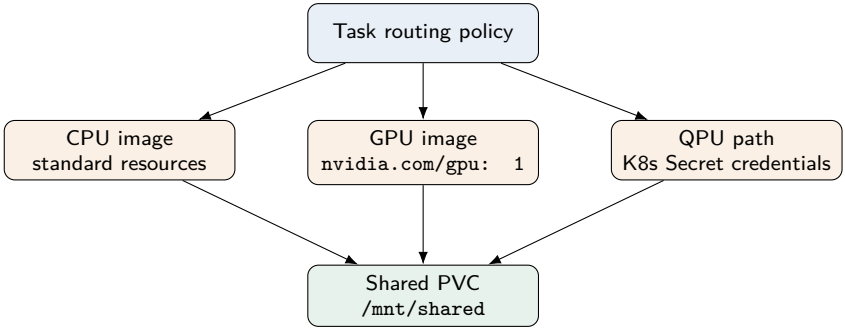

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Archived by the shared core

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Local convention

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Local checks

- compile the package and run smoke tests;
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- generate one SQD task and one Circuit Cutting task;
- verify that generated routing policies match UI choices.

Cluster checks

- upload kubeconfig from the UI;
- validate Argo, debug pod and shared PVC;
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Main message

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