Qanat

Experiment Tracking for HPC Users

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The Reproducibility Problem

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The Challenge

Existing tools (MLflow, Weights & Biases) require GUIs and databases, but HPC users work in **headless terminal environments** with job submission systems.

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- HTCondor/Slurm integration
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- Database servers
- Network connectivity
- Complex setup
- Heavy dependencies

Why Existing Tools Fall Short for HPC

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Qanat's Solution

A minimal, CLI-based experiment tracking system designed specifically for computational research on HPC systems.

What is Qanat?

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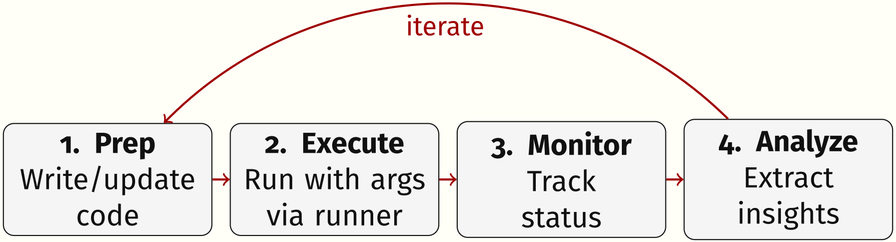
Qanat, version 1.9.4
Minimal experience management system.
```

- A tool I built for my own research needs
- Used by some students, but nothing groundbreaking
- Everything it does *can* be done without it
- Power users could write it in 50 lines of bash

So why use it? It enforces a structured workflow and handles the boring parts automatically.

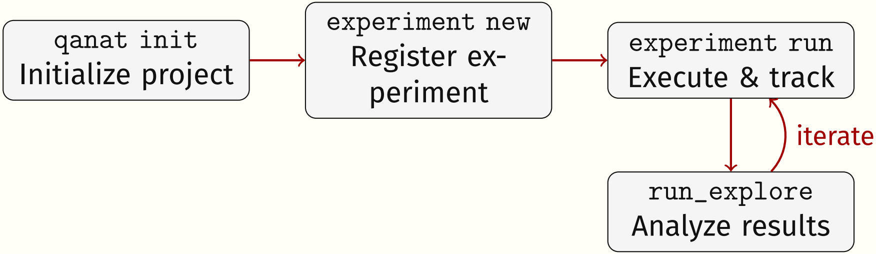
Overview

Standard steps in any computational experiment:



Qanat organizes these steps and forces you to work in a reproducible way.

The Experiment Lifecycle with Qanat



Automatic tracking: git commit, parameters, stdout/stderr, duration, status

Let's see qanat in action!

We'll demonstrate:

1. Initialize a project
2. Create a simple training script
3. Register an experiment
4. Run with parameters
5. Explore results interactively

Demo Note

Everything shown works the same on your laptop or on a 1000-node cluster.

For every run, qanat stores:

```
results/my_experiment/run_42/
|-- info.yaml              # All parameters + metadata
|-- stdout.txt             # Complete output
|-- stderr.txt             # Errors & warnings
`-- [your results]         # Whatever your script saves
```

info.yaml contains:

- Exact git commit SHA
- All command-line arguments
- Execution date, duration, status
- Tags, description, dataset links

Overview

Feature 1: Parameter Grid Sweeps

The Problem: Running experiments over multiple parameter combinations

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Qanat's Solution: Groups

- `-g` flag: Define parameter groups
- `-r` flag: Define ranges with start/stop/step
- Cartesian product between groups and ranges

Hyperparameter search across learning rates and seeds:

```
qanat experiment run train_model \
  --epochs 100 \
  -g "--lr 0.001" \
  -g "--lr 0.01" \
  -g "--lr 0.1" \
  -r "--seed 0 5 1"
```

Hyperparameter search across learning rates and seeds:

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```
results/train_model/run_17/
|-- group_0/  # lr=0.001, seed=0
|-- group_1/  # lr=0.001, seed=1
|-- ...
`-- group_14/ # lr=0.1, seed=4
```

Benefits of the groups concept:

- **Aggregation:** K-fold cross-validation, multiple random seeds
- **Organization:** Related experiments stay together
- **Efficiency:** Submit all variations in one command
- **Analysis:** Actions can operate on entire groups

Design Choice

Groups let you think about parameter *sweeps* rather than individual runs.

Runner Abstraction: Same command, different execution environments

Runner	Use Case	Backend
local	Laptop/workstation	subprocess
htcondor	HTCondor clusters	Python bindings
slurm	Slurm clusters	sbatch

Just add: `-runner htcondor`

Everything else stays the same!

HTCondor Note

Requires `htcondor` Python bindings `<11` (version 10.x recommended)

Submit to cluster:

```
qanat experiment run train_model \
  --runner htcondor \
  --submit_template gpu_template \
  -g "--lr 0.001" -g "--lr 0.01" -g "--lr 0.1" \
  -r "--seed 0 5 1"
```

Monitor progress:

```
qanat experiment status train_model --live
```

Qanat creates submit descriptions, tracks job status, and aggregates results automatically.

Reusable resource specifications:

Define once, use everywhere:

- CPU cores, memory requirements
- GPU requests (number, type)
- Docker/Singularity images
- Queue names, time limits

Example

`gpu_template`: Requests 1 GPU, 16GB RAM, cuda11.8 environment

Switch between small CPU tests and large GPU runs with just the template name.

Reproducible environments with Singularity/Apptainer:

- `-container path/to/image.sif`
- Automatic bind mounting of working directory
- Dataset paths mounted automatically
- GPU support via `-nv` flag
- Works with both local and HPC runners

Reproducibility++

Container + git commit = exact code *and* exact environment.

Container Example

```
# Run in container on cluster with GPU
qanat experiment run deep_learning \
  --runner htcondor \
  --container /shared/images/pytorch.sif \
  --gpu True \
  -g "--model resnet50" \
  -g "--model efficientnet" \
  -r "--batch_size 16 64 16"
```

Qanat handles:

- Bind mounting code and data
- GPU passthrough (`-nv`)
- Submit description generation
- Tracking container path in metadata

The most important feature: Qanat refuses to run uncommitted code!

Enforced Reproducibility

If your code isn't committed, your experiment isn't reproducible. Period.

Every run automatically tracks:

- Exact git commit SHA (e.g., `a3f4b2c`)
- Branch name
- Repository remote URL
- Working directory state

This is the foundation that makes everything else meaningful.

Qanat handles git checkout automatically!

Scenario 1: Exact reproduction

```
# Reruns with same commit + same parameters
qanat experiment rerun my_experiment 42
```

Scenario 2: Old code, new parameters

```
# Check which commit was used
qanat experiment run_explore my_experiment
# Shows: git_commit: a3f4b2c

# Run with that commit + different parameters
qanat experiment run my_experiment \
  --commit_sha a3f4b2c \
  --new_param value
```

Reproducing Experiments]Reproducing Experiments

No manual git checkout needed! Qanat does it for you.

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- Receive `-storage_path` automatically from qanat
- Access all files saved during the run
- Generate plots, compute metrics, export data
- Can be run from CLI or interactive menu

Feature 5: Actions for Result Analysis

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Benefit: Separate computation from visualization. Run experiment once, analyze many ways.

Define action in experiment YAML:

```yaml
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Action script structure:

```python
import argparse, numpy as np, matplotlib.pyplot as plt

parser = argparse.ArgumentParser()
parser.add_argument("--storage_path", required=True)
args = parser.parse_args()

# Load results from storage_path
results = np.load(f"{args.storage_path}/metrics.npz")
plt.plot(results['train_loss'], label='train')
plt.savefig(f"{args.storage_path}/learning_curves.png")
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Execute: `qanat experiment action my_exp plot_curves 42`

Real-time experiment monitoring:

- **TQDM integration:** Training loops show progress bars
- **Count format:** `Progress: 42/100` for parallel jobs
- **Group aggregation:** See progress across all parameter combinations
- **Live dashboard:** `-live` flag for auto-refreshing status

Implementation

Your script writes progress to stdout in recognized formats. Qanat parses and displays it.

Simple C program with parallel processing:

```
# Run with different thread counts
qanat experiment run montecarlo_pi --n_trials 10000000 \
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Plot action (gnuplot):

```
qanat experiment action montecarlo_pi plot 42
```

Creates convergence plot + random sampling visualization

PyTorch training with TensorBoard:

```
# Compare CNN vs pretrained EfficientNet
# Each experiment has its own dedicated script
uv run qanat experiment run mnist_cnn \
  --epochs 10 --lr 0.001 \
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- TensorBoard logs: Saved to `storage_path/tensorboard/`
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Why Bother Using It?

If you can do this in 50 lines of bash, why use qanat?

- **Enforces discipline:** Forces git commits, no shortcuts
- **Handles boilerplate:** Job submission, directory creation, logging
- **Consistency:** Everyone on your team uses the same structure
- **Lower barrier:** Students don't need to be bash experts
- **Documentation:** Forgot how something works? Check old runs

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Reality

It's just organized file management and script wrappers. Nothing revolutionary, but it saves time.

Overview

What qanat is:

- A personal tool I made to stop losing my own experiments
- Used by a few students in my group
- Open source on GitHub (AGPLv3)
- Maintained when I need new features

What qanat is NOT:

- Not polished or well-documented
- Not feature-complete (Slurm support is half-baked)
- Not tested beyond my own use cases
- Not a replacement for proper experiment management systems

Reality

It works for what I need. Might work for you. Might not. Your mileage may vary.

Limitations & Future Work

Known limitations:

- Slurm support still in development
- Interactive menu requires Linux/macOS (no Windows support)
- SQLite database limits concurrent writes
- No built-in visualization dashboard

Potential improvements:

- Better dataset versioning
- Experiment comparison tools
- Integration with Jupyter notebooks
- Enhanced action system

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5. **Nothing revolutionary:** Just organized wrappers, but that's often enough

Bottom Line

If you're already disciplined with git and bash scripts, you don't need this. If not, it might help.

Documentation & Code:

- **Documentation:** `https://ammarmian.github.io/qanat/`
- **GitHub:** `https://github.com/ammarmian/qanat`
- **Installation:** `pip install git+https://github.com/ammarmian/qanat`

Questions?

Feedback and contributions welcome!

Thank You!

Happy experimenting on your HPC clusters

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