



# Advancing Scientific Job Dispatch: Core Modernization, Cloud Integration, and Visual Workflow Tooling for k-Dispatch

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## 1 Origin: Precision Neurostimulation

**k-Plan** is a leading planning environment for **Transcranial Ultrasound Stimulation (TUS)**. It leverages the **k-Wave** acoustic toolbox to simulate ultrasound propagation through the human skull. To handle the massive computational cost of these simulations, k-Dispatch was created as a specialized middleware to bridge the gap between the desktop application and remote HPC clusters.



## 2 The Challenge: Complex Scientific Computing

Modern research requires massive compute power, but using it effectively is difficult:

### Technical Complexity

Managing **SLURM/PBS** scripts and cluster settings is hard. Researchers must manually tune parameters to balance **execution time vs. cost**.

### Limited Resources

Local workstations are often too slow, yet moving jobs to **HPC centers** or **Cloud** is technically demanding.

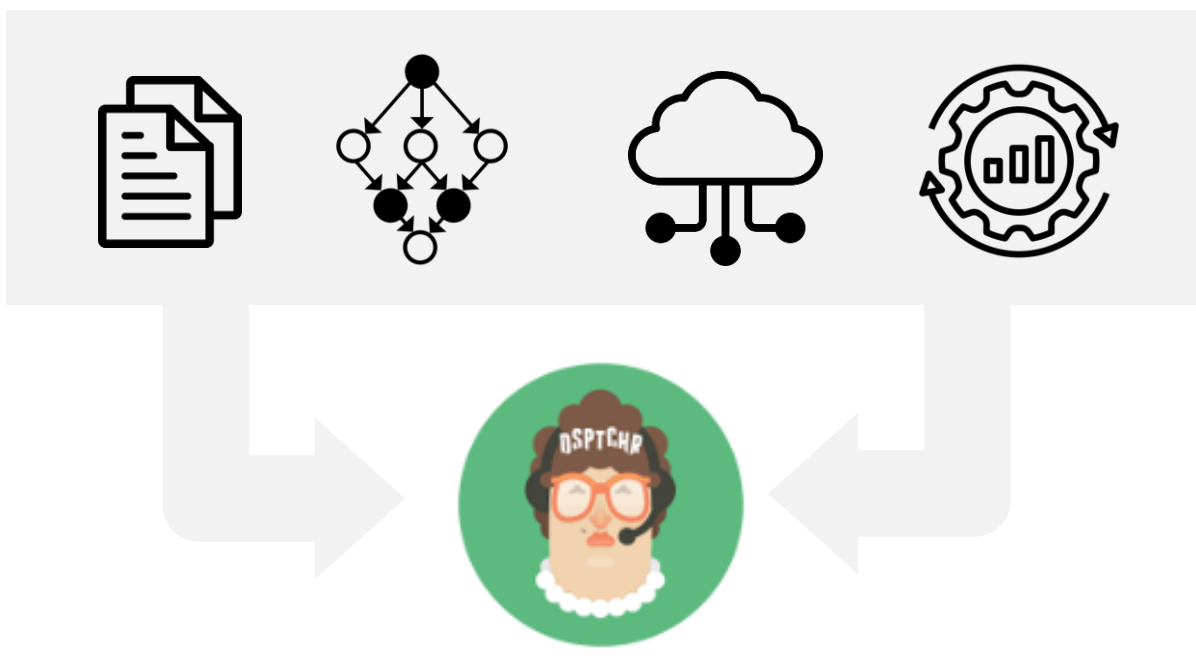
### Workflow Gaps

There is a lack of simple, visual tools to build, run, and monitor multi-step tasks without manual coding.

## 3 The Solution: k-Dispatch Modernization

This work presents the evolution of **k-Dispatch** from a specialized backend into a **domain-agnostic, modular middleware**. By introducing a modernized execution core, seamless **Microsoft Azure** integration, and a new **Visual Workflow Tool**, we lower the barrier to entry for high-performance computing across all scientific domains.

### Robust & Cluster-Aware



A modernized, modular execution core built for **smart scheduling, secure containerization**, and advanced **system observability**.

#### Smart Scheduling

New **Orchestrator** and **Optimizer** modules evaluate workflows in real-time. Execution is optimized based on a performance database and current cluster utilization.

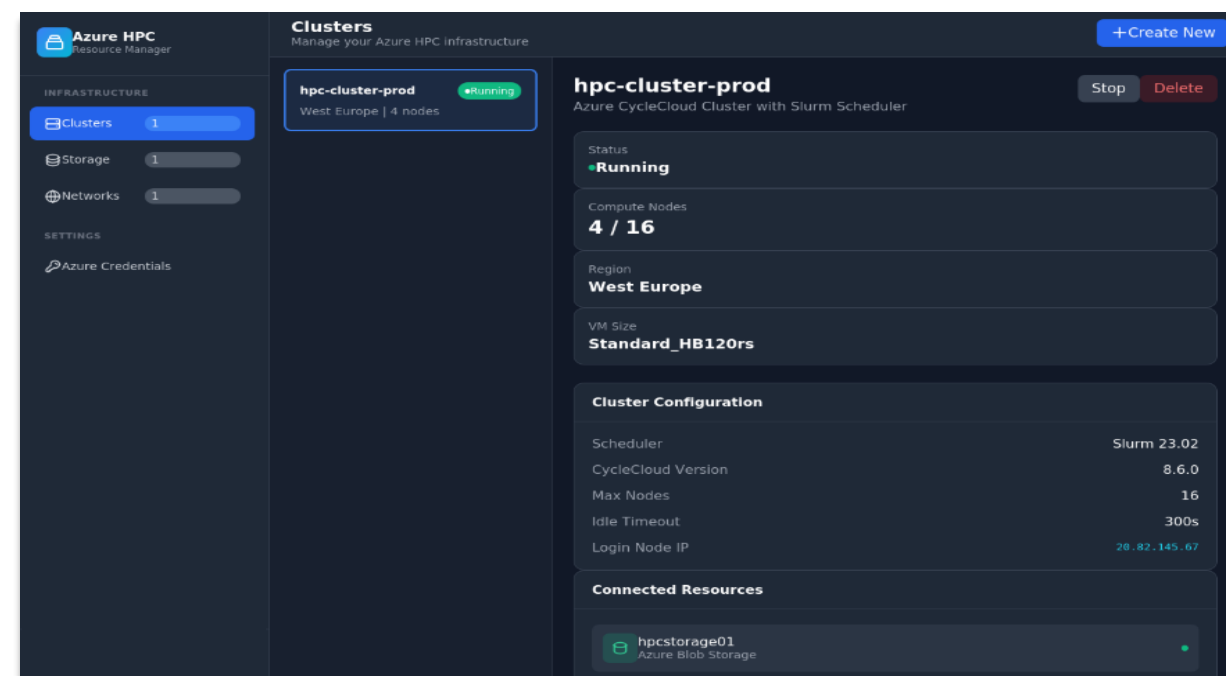
#### Modular Architecture

Designed for extensibility, allowing for easy integration of **new workflows, remote machines**, and **custom optimization strategies**.

#### Advanced Observability

Integrated **Loki** and **Grafana** to provide powerful log storage, parsing, and visual monitoring of the entire ecosystem.

### Cloud Integration



Extending k-Dispatch with a dedicated **Microsoft Azure** backend for **elastic scalability**.

#### Zero-Config Cloud

Users can offload workloads to **Azure CycleCloud** without writing specialized cloud-init scripts.

#### Automated Control

k-Dispatch handles all **job submission and monitoring**, ensuring a hands-off experience from start to finish.

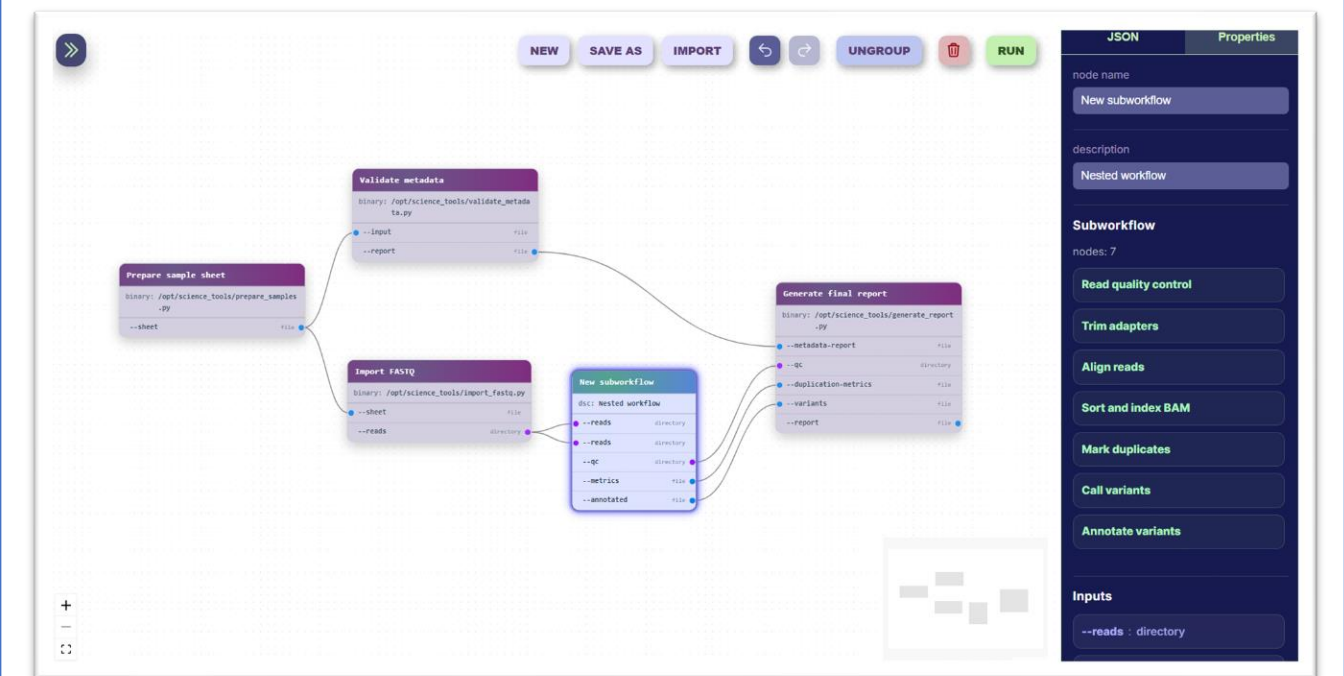
#### Elastic Cloud Bursting

Seamlessly offload workloads to Azure when local **HPC resources are exhausted**.

#### Integrated Cloud Management

Use **k-CloudManager** to configure settings and export them directly to k-Dispatch.

### Visual Workflow Tooling



Standalone **graphical application** for visual workflow composition and computation offloading.

#### Drag-and-Drop Composition

Users can visually link computational steps, defining dependencies **without touching a terminal**.

#### Script Generation

Directly creates valid **SLURM, PBS**, or standard **Bash** scripts.

#### Seamless Remote Deployment

**One-click transfer** bridges the gap between local workstations and remote clusters, **automating data movement** and **job submission**.

#### Modular Task Encapsulation

Group complex operations into reusable subworkflows for **cleaner pipeline management**.

## 4 Conclusions: A Unified Scientific Ecosystem

By combining a **modernized execution core** with **visual tooling** and **seamless cloud integration**, k-Dispatch creates a single, unified environment for complex scientific research. This integration removes the technical burden of managing clusters and cloud resources, allowing scientists to focus entirely on their results. The result is a professional-grade platform that balances performance, cost, and ease of use in a one-click workflow.