




Cloud-Based Virtual Desktops for Reproducible Research

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Abstract

Reproducing computing environments become increasingly challenging in research, especially when compute-intensive scientific workflows require specialised software stacks, specialized hardware (e.g. GPUs), and interactive analysis tools. While traditional high-performance computing (HPC) systems offer scalable resources for batch processing, they don't easily support interactive workflows. On the other hand, workstations have fixed resources and face workflow deployment challenges because conflicts can occur when multiple tools and dependencies are deployed into the same environment. To address these limitations, we present cloud-based virtual desktop platforms, built on the desktop-as-a-service (DaaS) model, using a containerised, cloud-native approach.

Our platforms offer on-demand, customized desktop environments accessible from any web browser, with dynamic allocation of CPU, memory, and GPU resources for efficient utilization of resources. We introduce two types of virtual desktops: BAND, built on top of a Slurm scheduler and BARD, using Kubernetes. In both cases, containerization ensures consistent and reproducible environments across sessions and pre-installed software improves accessibility for researchers. Deployment and system administration are also simplified through the use of orchestration and automation tools.

Our virtual desktop platforms are particularly valuable for bioimage analysis, which requires complex workflows involving high interactivity, multiple software and GPU acceleration. By combining containerization and cloud-native services, BAND and BARD offer a scalable and sustainable model for delivering interactive, reproducible research environments.

Keywords: cloud, virtual desktops, bioimage analysis

Resources

BARD desktop

- Code repositories:
 - Deployment and configuration: <https://github.com/embl-cba/bard-deployment>
 - Application containers: <https://github.com/embl-cba/bard-containers>
- Public instance:
 - <https://bard-external.embl.de>

BAND desktop

- Code repository:
 - Deployment: <https://github.com/embl-cba/band>
- Public instances
 - de.NBI: <https://bandv1.denbi.uni-tuebingen.de>
 - Euro-Biolmaging: <https://band.vm.fedcloud.eu>

Author contributions

YS: Conceptualisation, Software, Writing; **CT:** Conceptualisation, Writing - Review & Editing, Resources, Supervision, Project Administration, Funding acquisition; **HAK:** Software; **J-K H:** Conceptualisation, Writing - Review & Editing, Resources, Supervision, Project Administration, Funding acquisition

Competing interests

The authors declare that they have no competing interests.

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