

SimpleVM - a framework for federated research environments in the de.NBI Cloud

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Modern life sciences research has undergone a rapid development driven mainly by the technical improvements in analytical areas leading to miniaturization, parallelization, and high throughput processing of biological samples. This has led to the generation of huge amounts of experimental data. To meet these rising demands, the German Network for Bioinformatics Infrastructure (de.NBI) was established in 2015 as a national bioinformatics consortium aiming to provide high quality bioinformatics services, comprehensive training, powerful computing capacities (de.NBI Cloud) as well as connections to the European Life Science Infrastructure ELIXIR, with the goal to assist researchers in exploring and exploiting data more effectively.

Our de.NBI Cloud project type SimpleVM enables users with little to no background knowledge in cloud computing or systems administration to employ cloud resources with few clicks. SimpleVM is an abstraction layer on top of OpenStack to manage virtual machines (VMs) or clusters thereof. It was designed to support the combination of resources from independent OpenStack installations, thus operating as a federated multi-cloud platform which is accessible from a single web-based control panel. The entire software stack only requires access to 1) the OpenStack API and 2) an AAI provider (via Keycloak, LifeScience AAI) and it can be deployed on any vanilla OpenStack installation using Ansible. In general, SimpleVM primarily eases the creation and management of individual pre-configured virtual machines and provides web-based, SSO-protected access to popular research and development environments such as Rstudio, Guacamole Remote Desktop, Theia IDE, JupyterLab and Visual Studio Code. However, custom recipes based on Packer can be added to provide specific VMs tailored to user requirements.

A single SimpleVM project can host multiple VMs with individual access permissions for users. On top of this functionality, a dedicated SimpleVM Workshop mode streamlines virtual machine provisioning for workshops. Organizers can define a custom VM image and possible access methods, optionally based on the research environments mentioned above. When the workshop starts, participants can instantly access individual VMs based on this predefined configuration via ssh or browser. Once the VMs are ready, the system allows the organizers to automatically inform participants on how to access the resource.

Further, with SimpleVM, de.NBI Cloud users can effortlessly configure and manage their own SLURM-based BiBiGrid clusters with just a few clicks. This feature addresses the needs of researchers who want to run their tools or entire workflows across multiple machines and provides a simple route for users to learn how to use grid-based scheduling systems.

In summary, SimpleVM provides a comprehensive solution to bring federated, multi-cloud resources to end-users and in addition, provides a simple to use basis for online training and as an entry to grid-based computing.

Topic

Needs and solutions in scientific computing: Platforms and gateway

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