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Federated cloud computing enviroment for malaria fighting

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Impact

This is one of the first international experiences in which two Supercomputing Centers create a set using HPC Cloud computing and storage equipment distributed between the two institutions. For the connection of the centers used the network of academic research and RedIris, which provided the bandwidth necessary for the experience.

Overview

The research group of Dr. Hugo Gutierrez de Teran, Galician Public Foundation for Medical Xenómica (FPGMX) and member of Scientists Against Malaria, needed to perform, using different computational methods, virtual screening a chemical library of 350,000 chemical compounds original to study on a selected therapeutic target to further develop, based on the findings, new drugs against the parasite Plasmodium, which causes the disease.

A cloud computing collaboration with FCSCL, using the framework of the cooperation agreement signed months ago between the presidents of the regions of Galicia and Castilla-León was designed as the fastest way to solve this challenge.

Description of the work

The aim is to generate a list of potential candidate molecules to pass Bioassay in parallel using two independent methods of ligand-receptor coupling or docking. (In the field of Molecular Modeling, this is a method that predicts the preferred orientation of a molecule to be linked to another to form a stable complex. Knowledge of the preferred orientation in turn can be used to predict the strength of the association or the binding affinity between two molecules).

As part prior to this study, researchers from the group of Dr. Gutierrez de Terán generated a collection of possible molecular species for each of the chemicals, considering all the possible isomers (compounds with the same atomic composition but different structural formula) tautomers (two isomers that differ only in the position of a functional group) and protonation states (addition of a proton to an atom or molecule) which led to a collection 1,238.000 processed molecules. This type of calculation requires a large amount of computational resources, which can only be made using large datacenters.

CESGA technicians used the cloud developed in the framework of NUBA project, extending it to use resources from FCSCL. The management of both sites was performed using computer software developed in Spain, "OpenNebula", which manages the nodes in both locations, deploying virtual machines in either one or the other depending on the criteria of optimizing computing resources.

Conclusions

The collaboration between both supercomputing centers in the implementation of this cloud, in addition to being essential support in the development of international research groups, is a step in the research of technologies for cloud computing services, as it has generated Based on ongoing projects within the center itself. The success of the experience opens the door to new collaborations between national and international, which would meet very demanding computer applications for research projects almost immediately.

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