Introduction

Computational pharmacists nowadays have increasing demands both in using high-performance computing systems and in getting machine learning support. These users prefer high-level programming approaches with data science and visualisation support and find programming environments based on de-facto HPC standards (e.g., OpenMP and MPI) too complex and incomplete. Our HPC and web computing project builds a bridge between the worlds of accelerator-based HPC systems and data science enriched programming environments. Users specify problems in a Jupyter Notebook environment with possibly mixed Python and R sections that, depending on the computational load, can be executed either locally on a user workstation or remotely on an HPC system. As drug design will more and more depend on simulation, computational reproducibility will be a mandatory requirement, which our system fully supports.

Prototype System: High-Level Architectural View

The system is organized in three parts: A user interface (on the left) sending http requests to a web server (in the middle) that handles SSH connections to a remote system (on the right).

Re-using some of the components provided by PROVA! (web server and back-end), it is possible to implement HPC interfaces for different user categories.

The scientist uses JupyterHub to spawn and manage notebooks which are based on a specific container image (Docker/Singularity).

Use Case: Anomaly Detection in Lung Images

- **Problem:** Developing an algorithm to support clinical decision in lung cancer diagnosis detecting possible anomalies in the CT imaging of the lungs.
- **System:**
  - SW: Tensorflow 1.4.1, Keras 2.1.5
  - HW:
    - Roche EAA server: Nvidia K80
    - Microsoft Azure Cloud Platform: Nvidia P40
- **Method:** Convolutional variational autoencoder neural network[1].

![](Image)

Figure 1: Detection produced by the neural network

Platform Evaluation

- **Survival prediction of cancer patients**
- **Parkinson’s disease diagnosis**
- **Stochastic optimization for SCM**
- **American Option Pricing**
- **Stencil compilers benchmark**

References