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Design and implementation of a service for performing HPC computations in cloud environment

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Workflow of scientific computations

1. Group of scientists needs to perform computations
2. Application is being developed (usually by their own effort)
3. Then it’s being ported for execution in cluster environment
4. The same version is executed many times with different inputs

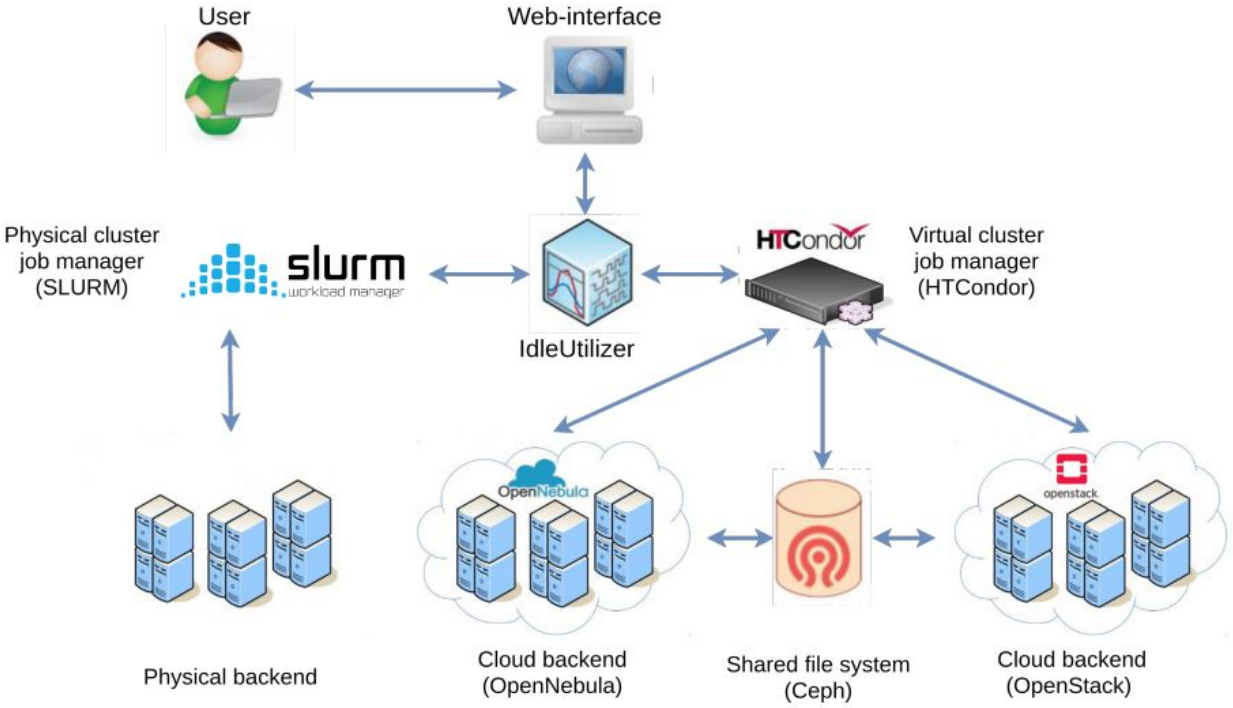
HPC and cloud computing

When operating in clouds it brings the following problems:

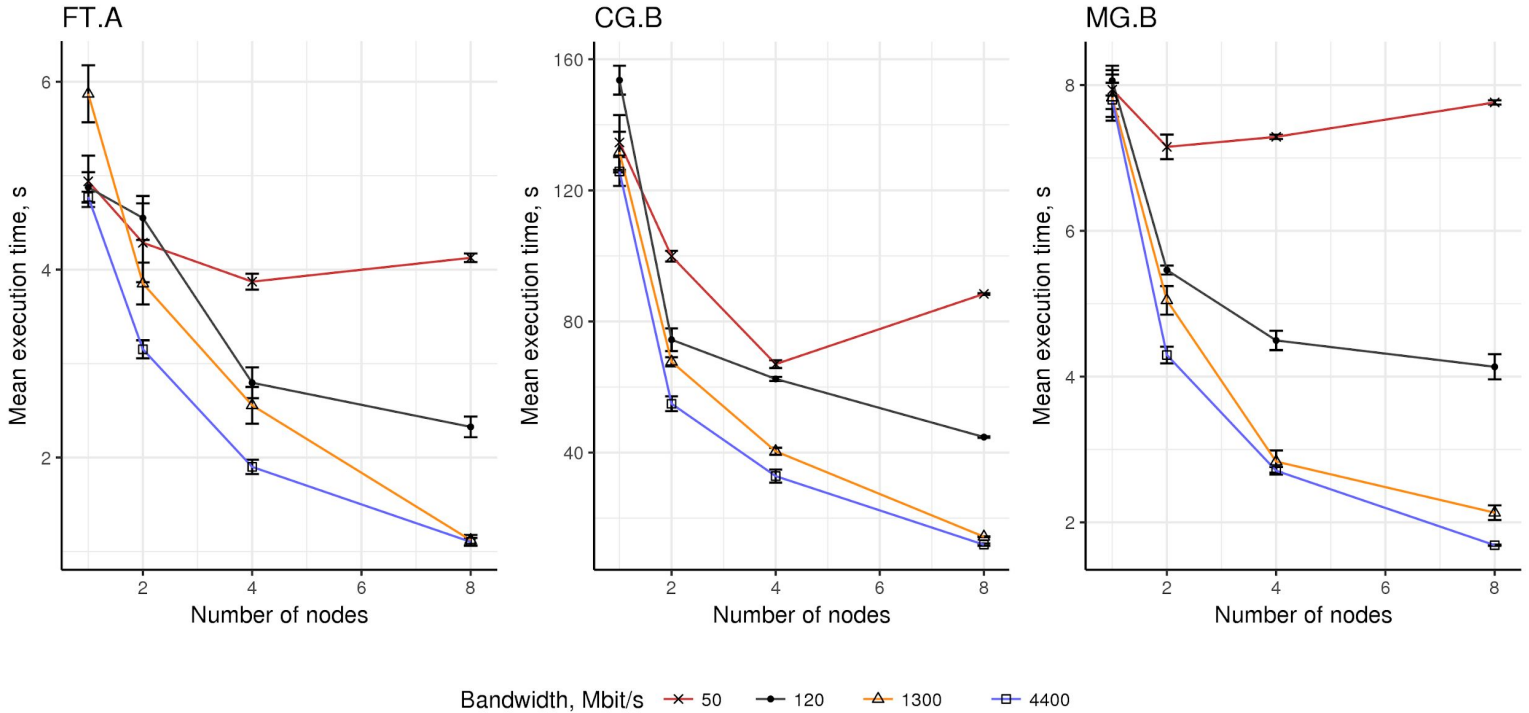
- A new virtual cluster has to be created for every application
- Somebody has to configure it to execute specific application
- Using an application happens in a weird way (for non-IT person), e.g.:
  - Find the address of the correct VM
  - Connect to it through VPN server via SSH
  - Setup environment, copy input data, launch application on correct VMs, copy the results back
  - Everything happens through command line interface
- Cluster configuration may be not optimal (too expensive or ineffective)

Scientists would rather focus on the problems in their field than spend their time configuring virtual machines.

Service architecture



Experiments



Cluster configuration optimisation problem

- y – discrete vector of cluster configuration (# of nodes, threads, memory)
- x – user task parameters
- $t = t(x, y)$ – task execution time
- $y^* = y^*(x) : t(x, y^*) \longrightarrow min$ – optimal cluster configuration

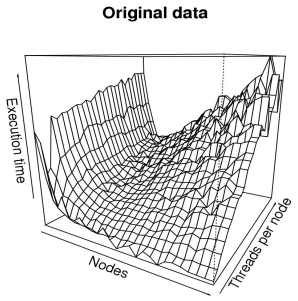
The problem is to create regression model for predicting y^* as a function of x

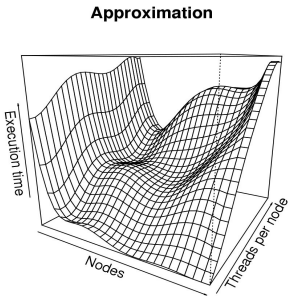
Method of cluster configuration optimisation

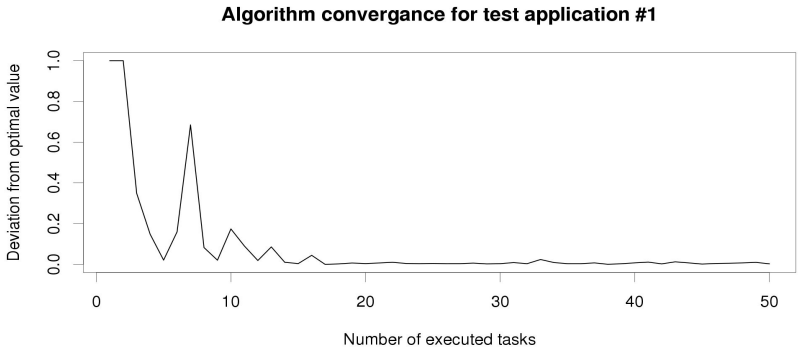
y^* is estimated by the sequence $\{y_n\} \rightarrow y^*$

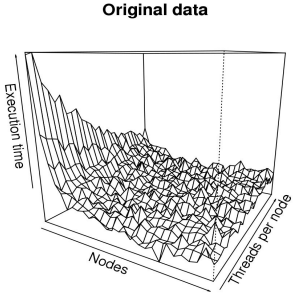
- Instead of optimisation of target function, its approximation with Fourier series is optimised (based on DONE optimization algorithm)
- Approximation is fitted to the data from the previous executed tasks with nearest input parameters (x)
- To find a global minimum gaussian noise is added to the estimates at each step

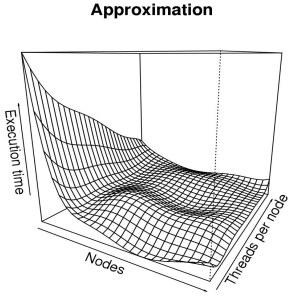
Method of cluster configuration optimisation

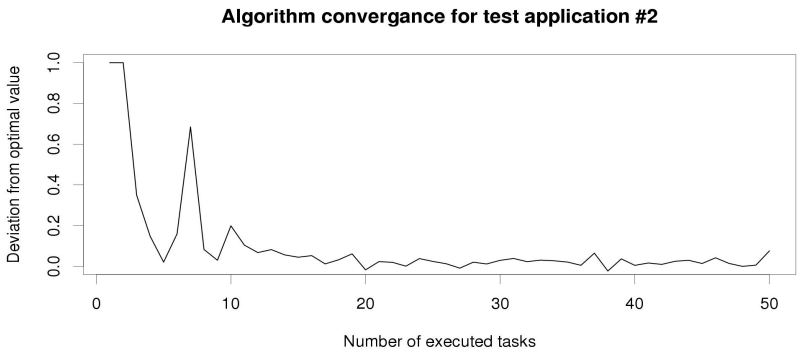












Conclusion

- In this work we've attempted to simplify the process of running HPC applications in cloud environment by
  - Automating virtual cluster configuration process
  - Providing users with a simple interface for submitting computational tasks
  - Optimising cluster configuration to reduce task execution time
- Software system has been designed, developed and tested in cloud environment
  - Right now it is used in a cloud of Nuclear Institute for the Nuclear Research for modeling long josephson junction
- Proposed a method for automatic cluster configuration and its prototype has been tested on synthetic loads

Research has been supported by the RFBR grant 16-07-01111.

Thank you for attention!