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Automation of Distributed Scientific Computations with Everest

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The report discusses common problems associated with the automation of scientific computations, as well as promising approaches to solving these problems based on cloud computing models. The considered problems include running computations on HPC resources, integration of multiple computing resources, sharing of computing applications, combined use of mutliple applications and running parameter sweep experiments. Due to the inherent complexity of computing software and infrastructures, as well as the lack of required IT expertise among the researchers, all these actions require a significant amount of automation in order to be widely applied in practice.

The use of service-oriented approach in scientific computing can improve the research productivity by enabling publication and reuse of computing applications, as well as creation of cloud services for automation of computation processes. An implementation of this approach is presented in the form of Everest cloud platform which supports publication, execution and composition of computing applications in a distributed environment.

Everest follows the Platform as a Service model by providing all its functionality via remote web and programming interfaces. A single instance of the platform can be accessed by many users in order to create, run and share applications with each other without the need to install additional software on their machines. Any application added to Everest is automatically published both as a user-facing web form and a web service. Unlike other solutions, Everest runs applications on external computing resources connected by users, implements flexible binding of resources to applications and provides an open programming interface. The implementation of the platform, application use cases and future research directions are discussed.

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