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AEGIS CMPC Scientific Gateway

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Description of Work

The earlier used interface to DCIs within the Serbian Condensed Matter Physics Community (CMPC) was based on gLite technology maintained by the European Middleware Initiative (EMI). The usage of computing resources provided through this technology requires a personal certificate from a Certificate Authority, Virtual Organization membership, and access to a User Interface machine. From user's perspective, this approach demands several skills: the knowledge of CMPC applications source codes and their parallelization, the knowledge of different compiler technologies, the knowledge of Linux operating system and its common tools, and the knowledge of gLite command line interface and DCI technology. Due to the complexity of applications used by the CMPC community, even with the set of self-developed scripts to control application process workflow, the desired level of automation was not achieved.

With the introduction of a generic-purpose Liferay-based WS-PGRADE/gUSE gateway technology (provided by the SCI-BUS project), we have been granted with the workflow interface, which was able to wrap complex execution diagrams of individual applications into single workflows. Developers have become able to create workflows using a user-friendly interface, while the users have become able to produce results in a much simpler way, by submitting the description of the physical system through a configuration file.

Transition to the WS-PGRADE/gUSE technology started with the deployment of a portal-dedicated VO (cmpc.aegis.rs) that was crucial for faster execution of jobs submitted from the scientific gateways, but also important for lobbying at the resource providers for additional or new resources. This has been followed by the installation of the generic-purpose Liferay-based WS-PGRADE/gUSE gateway (http://sci-bus.ipb.ac.rs:8080/liferay-portal-6.1.0/), its customization, and creation of CMPC application-specific workflows. Currently, the system supports workflows of three applications mainly utilized by the CMPC community: SPEEDUP, QSPEEDUP, and GP-SCL. SPEEDUP and QSPEEDUP applications use the similar algorithm, but rely on different random number generators, for calculation of quantum mechanical transition amplitudes for 1D models. This property, in combination with WS-PGRADE/gUSE features, allowed development of a common workflow for both applications. The third application, GP-SCL, solves the time-dependent Gross-Pitaevskii equation in one, two, and three space dimensions in a trap using imaginary-time and real-time propagation. The workflow of this application uses configurations provided by the users, to produce visualization of the dynamics of dilute trapped Bose-Einstein condensates.

User-defined configurations of physical systems, together with the results coming from the executed workflows, are stored in a document-oriented database (CouchDB). On top of this, a set of RESTful web-services enable end-users to provide new physical system configurations or to retrieve the produced scientific results. In addition, a user-dedicated web interface allows querying of stored configurations and results.

Printable Summary

Numerical simulations in the condensed matter physics deploy a broad range of algorithms, such as solving of nonlinear partial differential equations, classical and quantum Monte Carlo techniques, including solving of Bose-Hubbard and Fermi-Hubbard models, exact diagonalization techniques for strongly correlated systems, etc. Whichever is used, typically it requires large-scale computing resources for simulations of relevant physical systems.

Within the Serbian Condensed Matter Physics Community (CMPC), the most prominent use of computing resources is related to the three applications: GP-SCL, SPEEDUP and QSPEEDUP. The first one solves Gross-Pitaevskii equation, the effective equation governing the dynamics of Bose-Einstein condensates and nonlinear optical systems. The application solves both time-dependent and time-independent Gross-Pitaevskii equation in one, two, and three spatial dimensions using imaginary-time and real-time propagation. The SPEEDUP application uses Monte Carlo, while QSPEEDUP uses quasi-Monte Carlo-based path integral algorithm for calculation of quantum mechanical transition amplitudes and partition functions for 1D models.

Recently, within the framework of the SCI-BUS project and using the infrastructure of Academic and Educational Grid Initiative of Serbia (AEGIS), we have provided a Scientific Gateway on top of these three applications. The development relies on a widely utilized Liferay-based WS-PGRADE/gUSE portal, which was extended with the application-specific workflows, and a set of modules which enable specification of the physical system to be studied numerically, as well as exporting of the results of simulations.

This contribution illustrates the development and implementation of the AEGIS CMPC Scientific Gateway and main technologies used. We also briefly describe main workflows and present plans for further development.

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