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KIAM JOB_CONTROL TASK MANAGEMENT SYSTEM AND ITS APPLICATION TO THE CLOUD AND GRID COMPUTING

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Nowadays, the tasks related to development of nanotechnologies are of a great interest. The solution of such tasks requires the application of high-performance computing systems. Those computer systems are very expensive in installation and service therefore it is important to reduce the amount of their idle time. Due to this fact, the task of redistribution of calculations and restarting the applications on other available computing systems became a challenging problem for the systems end-users. In this work we provide a web-environment for carrying out mass supercomputer calculations. Throughout this work the KIAM Job_Control service was developed for controlling the applications and computing resources. KIAM Job_Control allows to perform long-term calculations on a set of supercomputers by automatic transfer of applications and calculated data between them. Basic functions of the system: application launch, application termination, data saving, relocation of save point on other supercomputer, application restart, interactive communication with the application during computation. The KIAM Job_Control service is designed to deal with a wide variety of tasks. The GIMM_NANO software complex oriented on the solution of actual tasks of nanotechnologies works using this service. One of applications is a module for molecular dynamics calculations. By means of this module multiscale simulation of non-linear processes in gas-metal microsystems is made. In the presentation we will describe the technologies allowing to realize the required service functionality. Also an example of its usage will be presented on the tasks of molecular dynamics calculations. The work was supported by Russian Foundation for Basic Research (projects 15-07-06082-a, 15-29-07090-ofi_m).

Primary author: Mr PUZYRKOV, Dmitry (Keldysh Institute of Applied Mathematics)

Co-authors: Prof. IAKOBOVSKII, Mikhail (Keldysh Institute of Applied Mathematics); Prof. POLYAKOV, Sergey (Keldysh Institute of Applied Mathematics); Dr PODRYGA, Viktoriia (Keldysh Institute of Applied Mathematics)

Presenter: Mr PUZYRKOV, Dmitry (Keldysh Institute of Applied Mathematics)

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