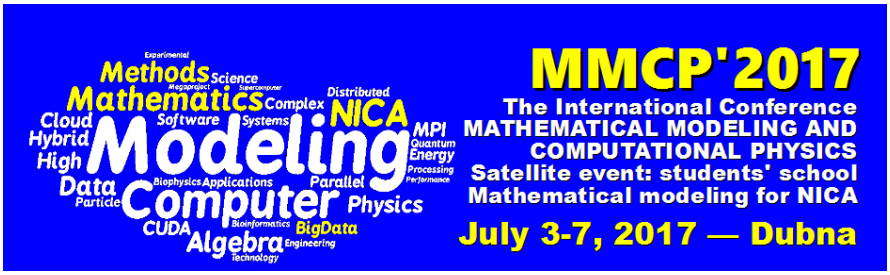

Contribution ID: **123** Type: **not specified**

Concept of a cloud service for data preparation and computational control on custom HPC systems in application to molecular dynamics.

Tuesday, 4 July 2017 14:30 (15 minutes)

The development of computer technology greatly expanded the possibilities of computational experiment. At the present stage it is already possible to study the properties and processes in complex systems at the molecular and even atomic level, for example, by the means of molecular dynamics (MD). The most interesting are problems related with the study of complex processes under real physical conditions.
Solving such problems requires the use of high performance computing systems of various types, for example, GRID systems and HPC clusters. For parallel calculations using the MD methods it is necessary to create an initial structure of computational domain, which describes the starting conditions, types and properties of the particles involved in the simulation.
Also, considering long-time computational tasks, there is a need for software of automatic monitoring such tasks and data relocation from HPC to the user storage.
Most of these actions today a scientist performs manually.
Authors will present the concept and the prototype of cloud service KIAM MolSDAG, intended for design of atomistic systems of large volume for further detailed molecular dynamic calculations. The main objective of the service is to provide a user the interface for designing an atomistic structure and then the preparation of input data for its numerical analysis using a variety of MD simulators. The second task of this service is to deploy, monitor and relocate the calculation-related data on the user-defined HPC system.
The individual elements of the service have already been implemented and confirmed the effectiveness of the overall service concept.

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Session Classification: Distributed and parallel computing and tools for scientific computing (I)