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Scientific and Engineering Workflows Based on Grid Services Orchestration

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The interdisciplinary CAE/CAD software able to solve problems of high complexity and with desired accuracy at the reasonable simulation time are of high demand today. The multi-layered architecture of the grid-enabled computer simulation software GridALLTED combining the benefits of distributed computing and SOA with workflow management capabilities has been proposed and successfully implemented. The basic idea of the proposed solution is the dynamic composition of both web and grid services for the execution of custom simulation scenario as a workflow. Workflow is executed as the orchestration of SOAP web services representing the basic building blocks of system's functionality: input data preprocessing; automatic mathematical model creation and its reduction; DC, AC, TR and sensitivity analysis; parametrical optimization etc. Compute-intensive steps are implemented as grid services interacting with the resources of Ukrainian grid infrastructure to run computations. The prototype of this system has been deployed at the resources of the HPC Centre of the NTUU “KPI”. Its further development is connected with the utilization of cloud resources.