Programming and Execution of Multiscale Applications

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1. Introduction

In this paper we describe a multiscale programming and execution framework developed in the MAPPER project. We aim at applications that can be built from single scale models and are described in the Multiscale Modeling Language (MML) [1]. The framework supports composition and execution of multiscale applications from existing single scale submodules installed on e-infrastructures [4,5]. It consists of a tool for application composition called Multiscale Application Designer (MAD), an application module description registry – MAPPER Memory (MaMe), the GridSpace (GS) supporting execution of applications in various infrastructures and Provenance Tracking System supporting result management.

2. Description of the framwork

The architecture of the framework is presented in Fig. 1.

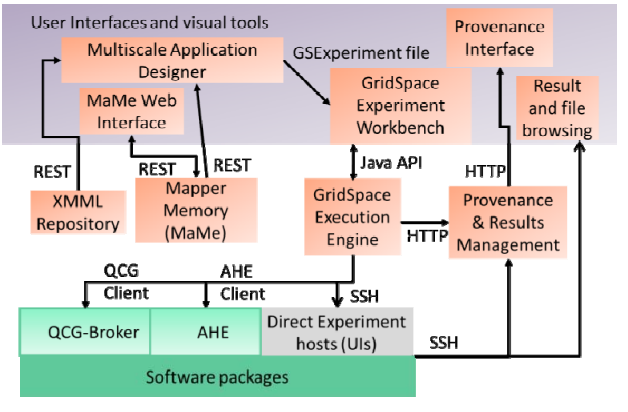

Fig. 1. Architecture of programming and execution tools. The user registers single scale modules in MaMe, composes them in a multiscale application in MAD and executes in GridSpace.

MAD supports applications' composition using a graphical form of MML and transforms it to executable GridSpace Experiment. MaMe is a registry for MML-based descriptions of single scale application models used in the composition step supported by MAD. xMML

Repository stores XML format of MML (xMML) of applications and provides them to MAD for reusability. GridSpace [3] supports high level stage of execution and interacts with underlying interoperability layer: Application Hosting Environment (AHE) and QCG-Broker to access the infrastructures. Result Management is a part of Provenance system that is able to save snapshots of experiment results together with their metadata, so a user is able to view experiments results and their metadata using Provenence Interface. The tools are web based services available on-line[1]

3. Results

During the MAPPER school[2], we have measured tools usability [2]. The obtained average SUS score was 68 points (for 100 possible); with standard deviation 18. The average was calculated from answers of 10 the most active participants. We applied our tools to the physiology [1], irrigation canals application[2], to simulation of clay-polymer nanocomposites (nanomaterial science), reverse engineering of gene-regulatory networks (Computational Biology), equilibrium-stability and transport turbulence equilibrium workflows (Fusion modeling). At present 20 single-scale models and 25 mappers used to translate data between models are already registered in the MaMe, representing all MAPPER applications.

4. Conclusions and future work

We conclude that the proposed environment has proven to be useful and can help scientists to develop different applications from a single set of modules. Web interface enables sharing applications modules among scientists working on the same area. Additionally, support for interactivity is provided.

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