Modelling of Simulation Workflows
Dipl.-Inf. Polina Malets, Jun.- Prof. Dr. Dimka Karastoyanova, Prof. Dr. rer. nat. Frank Leymann
Institute of Architecture of Application Systems (IAAS)

Motivation
In this project, we investigate the use of the workflow technology [1] for scientific simulations. We create a meta-model for simulation workflows and develop a graphical tool that scientists can use to model their workflows. The workflow technology provides multiple benefits:

- more coarse-grained granules of reuse like newly defined fragments, for example, to speed up the creation of simulation workflows
- robustness of the long-running simulation workflows: a failure of an individual step in a simulation should not result in the need to rerun the complete simulation
- automated and distributed execution
- simplified integration of IT execution

State of Current Work
In order to meet the requirements of scientists we have developed following concepts and approaches for the modelling of simulation workflows:

- Simulations with Shared Context
  - A simulation scope packages common context information of multiple simulation workflows and other shared data.
  - Enables support for multi-scale and multi-physics simulations with sequential and parallel simulation runs.
  - Synchronization and coupling mechanisms for multi-scale and multi-physics simulations in order to associate multiple simulation models corresponding to one common, real world phenomenon.

- Choreography
  - Enables data exchange between multiple simulations workflows.
  - The changes in one simulation can be immediately adopted in the other one, while the involved processes are running.
  - Choreography definition for multi-scale and multi-physics simulations.

- Data Management
  - With data references [3] the transfer of huge amounts of data through the workflow engine can be avoided. Data is passed directly to where they are required, while no relevant information is lost.
  - Data management activities enable an unified access to heterogeneous external data in simulation workflows.

- Support for Data Stream
  - Support and integration of stream data from various sources with heterogeneous formats and frequency.
  - Extension of workflow meta-model defining modelling constructs for stream processing, e.g. filtering, synchronization, disaggregation of data streams.

Connection to the SimTech Vision
The novel modelling approaches for simulation workflows leverage the benefits of the existing workflow technology and provide for an intuitive and straightforward simulation workflow development. These approaches can be considered as enablers for integrative science on the IT level.

Prototype
We have designed and implemented a subset of the concepts for the modelling of simulation workflows:

- Architecture and prototype of modelling tool with separate perspectives corresponding to each lifecycle phase of simulation process management [2]
- Integration of data management activities using data reference to deal with data intensive scientific experiments – both meta-modell and implementation level
- Extension of the workflow meta-modell and implementation of data management activities; service catalogue; data references; perspectives
- Extension of enterprise service bus for data streams processing

Future Work
In our future work:

- we will investigate, how interconnected simulations can be modeled, which existing modeling approaches for choreography are more suitable and how they can be adopted for certain types of scientific simulations
- we will pay attention to transaction mechanism and concurrent data access for interconnected, and in particular long-running simulations in order to achieve robustness and consistency in case of unforeseeable failures and to resume a simulation/experiment after a failure
- we will focus on seamless integration with monitoring, visualization legacy applications, so that an interactive framework is created

Cooperation
For the successful fulfillment of the tasks in our project we rely on cooperation within our network and with the other research network:

- PN 8, Institut of Architecture of Application Systems (Dipl.-Inf. Katharina Görlich, Dipl.-Inf. Mirko Sonntag, Dipl.-Inf. David Schumm), Paper on the application of process views to scientific workflows
- PN 4, Institute of Mechanics (Dipl.-Ing. Robert Krause), Application examples for shared context in multi-scale and multi-physics simulations
- PN 6, Institute of Nuclear Technology and Energy Systems (Dipl.-Ing. Tudor Ionescu, M.Sc.), Application examples for using stream data in scientific simulations

References