

USING WORKFLOWS IN M&S SOFTWARE

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ABSTRACT

The usage of workflows to standardize processes, as well as to increase their efficiency and the quality of the results is a common technique. So far it has only been rarely applied in modeling and simulation. Herein we argue for employing this technique for the creation of various products in modeling and simulation. This includes the creation of models, simulations, modeling languages, and modeling and simulation software modules. Additionally we argue why roles should be incorporated into modeling and simulation workflows, provide a list of requirements for the workflow management system and sketch first steps in how to integrate workflows into the M&S framework JAMES II.

1 INTRODUCTION

M&S applications may incorporate diverse products. These products may comprise models (or model components), simulations (experiments with a model), (modeling) languages, or M&S software. The importance of following well defined processes to achieve these diverse products is not new to M&S. A number of *M&S life cycle models* have been proposed to help developing and interpreting validated and verified models (Balci 1990, Sargent et al. 2006, Law 2007). However, the quality of simulation studies does not only depend on validated and verified models but also on the underlying validated modeling and simulation methods (Himmelspach and Uhrmacher 2009b), which in turn might require extensive simulation studies, e.g., to experimentally validate the accuracy or superiority of a simulation method in comparison to others (Jeschke and Ewald 2008). Thus, to the final product, e.g., simulation results that confirm a hypothesis about the dynamics of a given system, diverse M&S “workflows” involving different users have contributed. Also in the light that currently, simulation faces a credibility crises (Pawlikowski et al. 2002, Pawlikowski 2003, Kurkowski 2006), the desire emerges for more documentation of and guidance through these processes.

Workflow systems are aimed at providing software support for documenting, executing, and controlling workflows. They facilitate determining and eliminating problems in a production process that might induce errors in the final product (van der Aalst and van Hee 2004). Well defined workflows are considered to be mandatory for a repeatable production process (ISO 9001:2008 2008); repeatability being a salient feature of any experimental science.

Thus, integrating workflow management systems in M&S processes would increase the quality of products and strengthen credibility. In concrete, possible benefits would be improved repeatability, means to track “product” creation stepwise, intuitive task description, auto documentation and progress information, and a far reaching automation of M&S processes.

In the following we will give a short overview on workflows in science and M&S, discuss two use cases to illuminate the need for flexible workflow support, introduce different roles according to different types of M&S users, use these use cases, roles, and a set of established requirements for workflow management systems to define requirements for M&S workflow systems, and finally, identify a few crucial steps toward realizing such a workflow system, illuminated by the example JAMES II.

2 WORKFLOWS FOR SCIENTIFIC PROCESSES AND M&S

Workflows are recently receiving more and more attention in the scientific domain. So it is not surprising that more and more workflow systems emerge that support scientific processes. Project Trident (Barga et al. 2008, Barga et al. 2008),

Taverna (Hull et al. 2006, Oinn et al. 2006), Kepler (Altintas et al. 2004, Ludäscher et al. 2006) to name just a few of such systems.

Depending on the specificity of the systems, different approaches are pursued in managing workflows. General systems as Project Trident, Taverna and Kepler allow the scientists to create their own workflows or to edit, enhance and reuse existing ones. Systems are developed to publish, share, store, and query scientific workflows and experiments, e.g., the so called myExperiment project (Roure et al. 2008) provides a repository for sharing research objects used by scientists, such as scientific workflows. It is also supported by Taverna (Roure and Goble 2009) and Project Trident.

While those systems are aimed to provide support for general scientific workflows including as in the case of Kepler support for specific M&S aspects by building on PTOLEMY II (Lee and Neuendorffer 2007, UC Berkley EECS Dept. 2010), other systems such as SYCAMORE (Weidemann et al. 2008), SWAN Tools (Perrone et al. 2008) and JAMES II (Himmelpach et al. 2008, Himmelpach and Uhrmacher 2009a) are dedicated toward supporting M&S processes.

JAMES II, SYCAMORE and SWAN Tools hide the workflow aspect by only supporting fixed predefined workflows that can be executed by the scientists to assist them.

JAMES II, e.g., provides predefined workflows to create a basic simulation experiment by guiding the scientist through the steps of selecting a formalism, creating, loading or editing a model, parameterizing the model, selecting a simulation algorithm and a visualization. This results in an experiment description that can be executed afterwards. Another predefined workflow in JAMES II is aimed at supporting the experimental validation of models. It refines the basic experiment workflow integrating additional steps to select the type of experiment (e.g., Optimization Experiment, Parameter Scan, Sensitivity Analysis, etc.) to be performed (Leye, Himmelpach, and Uhrmacher 2009).

SYCAMORE is a web based front end supporting, e.g., COPASI (Hoops et al. 2006) as simulation engine, different online resources like databases, and locally available tools. SYCAMORE provides a fixed workflow. It guides through the process of setting up a model by selecting kinetic data from a connected database, adjusting parameters, model checking, parameter estimation, sensitivity analysis, and simulation execution using COPASI. However, experiences with SYCAMORE have revealed that whereas novices appreciate this strict guidance more experienced users found the solution too restrictive and wished for workflows that balance guidance and sufficient flexibility for adaptations.

The SWAN Tools provide a web based framework for the automation of the entire simulation workflow with SWAN (Liu et al. 2001). It assists and guides the scientist when configuring models with parameters by using an information rich interface that should enhance the understanding of what each parameter does. It also helps the scientist to manage and create simulation experiments and their configuration by letting the user define data for simulation runs and also to select or provide a specific simulator. Additionally simulation runs are generated for the scientist and can automatically be distributed in, e.g., a cluster. The simulation results are provided via a database interface as well as using different visualizations.

3 USE CASES

This section focuses on presenting two potential use cases for workflows in the M&S systems like JAMES II. They form the basis to define requirements that are essential in a workflow system intended to provide support for applying and evaluating M&S methods. The former refers to typical simulation studies, in this case we focus on the phase of creating a model, the latter deals with the problem how simulation algorithms can be evaluated.

3.1 Creating a Model for Simulation

Usually process models for M&S found in literature (e.g., Sargent 2008, Balci 2004, Law 2007) are described at a rather abstract level and just contain general task descriptions like “create qualitative model”. This coarse grained description leaves a high degree of freedom for interpretation on how to execute each step but results in a hardly traceable process execution which makes it difficult to find potential sources of errors or to ensure specific requirements and therefore a specific quality. Thus, these steps need to be refined for realizing a suitable support via workflows.

The workflow in Figure 1 is based on the process model for model creation introduced in (Balci 1990). The process of creating a simulation model can be described by the following steps:

System Investigation The *System Investigation* deals with the investigation of system properties used for system definition and modeling. It also defines the simulation study’s *Objectives*, i.e., the questions to be answered. System properties are identified that are of relevance for answering those questions. Typically as part of *System Investigation* data are collected and relevant input parameters are identified.

Model Formulation During the *Model Formulation* step the system under study is described as conceptual model taking the previously identified *Objectives* and the resulting requirements into account.

Model Representation The *Model Representation* turns the previously formulated conceptual model into a communicative model. The communicative model allows other parties (Researchers, Project Lead, etc.) to comment and to discuss the model.

