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Coupling between a multi-physics workflow engine and an optimization framework

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ABSTRACT

A generic coupling method between a multi-physics workflow engine and an optimization framework is presented in this paper. The coupling architecture has been developed in order to preserve the integrity of the two frameworks. The objective is to provide the possibility to replace a framework, a workflow or an optimizer by another one without changing the whole coupling procedure or modifying the main content in each framework. The coupling is achieved by using a socket-based communication library for exchanging data between the two frameworks. Among a number of algorithms provided by optimization frameworks, Genetic Algorithms (GAs) have demonstrated their efficiency on single and multiple criteria optimization. Additionally to their robustness, GAs can handle non-valid data which may appear during the optimization. Consequently GAs work on most general cases. A parallelized framework has been developed to reduce the time spent for optimizations and evaluation of large samples. A test has shown a good scaling efficiency of this parallelized framework. This coupling method has been applied to the case of SYCOMORE (SYstem COde for MOdeling tokamak REactor) which is a system code developed in form of a modular workflow for designing magnetic fusion reactors. The coupling of SYCOMORE with the optimization platform URANIE enables design optimization along various figures of merit and constraints.

1. Introduction

Generic purpose workflow engines can be used to solve physics problems involving a number of coupled modular components. These generic purpose workflow engines usually lack numerical optimization tools, which are instead embedded in dedicated optimization frameworks. This work presents a generic coupling method between a multi-physics workflow engine and an optimization framework, thus enabling the optimization of complex simulations integrating potentially a large number of workflow components. This method has been successfully applied to the optimization of fusion reactor design.

The main objective is preserving the integrity of both frameworks. The solution is to separate them as much as possible in order to run them independently. They are coupled by an exchange of data as it is illustrated in Fig. 1. One waits for the data coming from the other to run and send its results to the other. Each framework sees the other one as a black box. The data communication is performed by a socket-based communication library called KUI (KEPLER–URANIE Interface) which we have developed for this purpose. Instead of a tight integration, the two frameworks remain loosely coupled with this socket-based communication. This coupling architecture allows thus to replace easily any scientific workflow or optimization algorithm by another one. Moreover, optimizer frameworks or workflow engines can be changed without affecting the coupling procedure.

Software and tools for both frameworks have been chosen for their simplicity of use and their adaptability to any physics context. The workflow engine chosen for the multi-physics framework is

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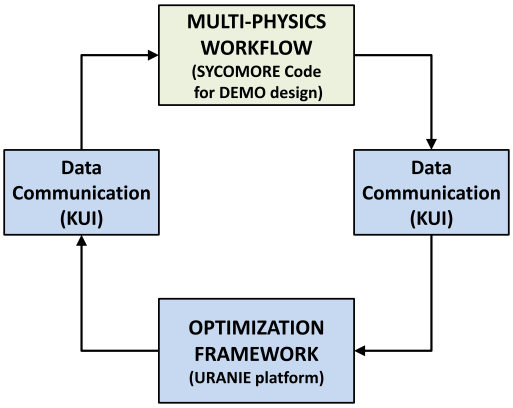

Fig. 1. The system code SYCOMORE for DEMO designing is coupled with the URANIE platform by using the socket-based communication library KUI.

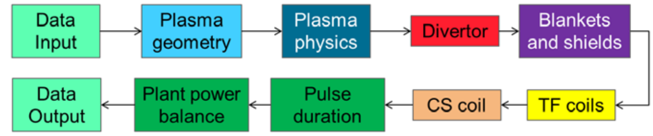

Fig. 2. Diagrammatic view of the SYCOMORE workflow with the series of subsystems components (CS = Central Solenoid, TF = Toroidal Fields).

the graphical software KEPLER [1,2]. A standardized data model adapted to the physics context ensures data consistency within the complete workflow. This facilitates the use and the development of workflows and gives more modularity. Optimizations are achieved by the URANIE platform developed by CEA. Such platform provides various tools for optimizations, data analysis and sensitivity studies. Genetic Algorithms (GA) have been selected to perform optimizations since they have demonstrated their efficiency. Such algorithms can achieve single and multiple criteria optimizations and they are enough robust to handle non-valid data which can appear during the optimization. Other tools provided by URANIE such as for data analysis and sensitivity study can be helpful to confirm optimization results or highlight parameters which mostly impact the optimum [3].

An external parallelized framework has been developed to speed up optimizations and evaluation of large samples. This parallelized framework has been demonstrated on up to 320 CPU on the EUROfusion Gateway cluster at the IPP Garching [4] hosting the European Integrated Modelling (EU-IM) platform. This architecture can be also generalized to grid computing.

A number of couplings between a code and an optimizer have been already achieved in the past. For instance the Computational Fluid Dynamics (CFD) code N3S-Natur has been coupled to the MIPTO optimization application by using the PALM coupler [5]. The latter one exchanges data by using MPI which is also a socket-based communication. Another example is the optimizer DAKOTA which has been coupled to the CFD code OpenFOAM [6]. DAKOTA and OpenFOAM exchange data by using files. The coupling proposed in this paper is similar to the one developed between the IPS and DAKOTA systems [7]. However, several main differences between the present work and the one described in [7] can be noticed. First, multi-physics workflows are developed on a graphical software (KEPLER) and use a standardized data model for the communication between workflow components. Second, the socket based communication is one of the solutions to allow a loose coupling between the two frameworks. The two platforms thus keep their integrity so that any change in one side (elements inside the platform or even the platform itself) will not affect the other one. This communication method also allows running the optimization framework and the workflow engine on different computers, thus potentially enabling distributed (grid/cloud) computing.

To illustrate the present coupling method, the modular system code SYCOMORE (SYstem COde for MOdeling tokamak REactor) developed by CEA to study DEMO fusion reactor design has been coupled to the URANIE platform. SYCOMORE aims at representing the interaction of main DEMO power plant subsystems from the central plasma to the power Balance of Plant [8]. Each reactor subsystem is represented by a component connected to the others in a KEPLER workflow. The inter-component exchange of data is performed by using the standardized data model developed by the former EFDA Task Force on Integrated Tokamak Modelling [9,10]. Here, optimizations achieved by URANIE aim to determine the best DEMO reactor design and highlight main technological developments required to get efficient fusion reactors. Several other system codes based on a different approach from SYCOMORE have been also developed to study DEMO design [11–13]. They are less modular and optimizations are more complex to carry out.

The current paper presents tools and methods developed to achieve the coupling between a multi-physics workflow engine and an optimization framework based on the SYCOMORE–URANIE coupling. The system code SYCOMORE and especially the architecture used for its development are presented in Section 2. This part also gives details on the characteristics of the data involved in SYCOMORE. Section 3 is dedicated to the KUI communication library. The URANIE tools are presented in Section 4. Especially, the URANIE genetic algorithm is described in this part since it is used to achieve SYCOMORE optimizations. Section 5 is focused on the parallelization procedure of SYCOMORE and its performance is assessed. Finally, some results of SYCOMORE sampling and optimization are shown in Section 6 in order to illustrate the performance of the SYCOMORE–URANIE coupling.

2. Multi-physics workflow frameworks

2.1. Modularity and graphical interfaces

The KEPLER software has been chosen by the EU IM framework to run workflows (e.g. SYCOMORE). It is a JAVA-based application for the analysis and modeling of scientific data [1,2] providing a graphical user interface which allows creating executable scientific workflows.

Each modular component of the scientific workflow represents an independent model and is called actor in KEPLER. Furthermore, several actors which are a part of a common sub-system can be gathered in one composite actor to make a coherent group of actors. The SYCOMORE system code is therefore a workflow which links together a series of components each representing a model of a reactor subsystem [8]. A diagrammatic view of the chain made of current components is presented in Fig. 2. In SYCOMORE, components are executed sequentially and each of them sends the computed data to the next one at the end of its execution. A few internal loops over several actors (included within composite actors) are introduced in order to let some parameters converge to specified values. The position of a component in the sequence is determined by its required input data (provided by previous components). Furthermore, the reactor design is built by radially integrating subsystems one after the other starting from the center of the plasma up to the edge of the reactor. This impacts the position of components in the workflow. It also allows thus to keep the design consistency.

The graphical organization of components makes the code structure easy to understand (see Fig. 3). This facilitates the collective development of an integrated modeling workflow. On the developer side, this helps contributors to see the sequence of components clearly and easily, as well as where their own

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