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Sequential parameter optimization for algorithm-based design generation using data from multiphysics simulations

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Abstract

The implementation of algorithmic modelling in CAD technologies is an opportunity to reduce manual design work in repetitive design tasks. This increases the importance of design automation and digital workflows. This technology can process the results from computational fluid dynamics (CFD) and finite element analysis (FEA) automatically and can optimize designed geometries sequentially. Nevertheless, this design process often sets high computational requirements. The aim of this paper is to present a design automation workflow that reduces the computational time of a design process. The computational resource requirements of the system are reduced by using knowledge-based engineering techniques to obtain information from previous successful designs, decomposing the design into sub-parts according to their functions and optimizing each sub-part individually. Furthermore, through algorithmic modelling, the different input geometries required for the physical description of each simulation are made separately. This allows different design simplifications to be made for each simulation domain. Once the output of the simulations is obtained, the design is evaluated in CAD to optimize the geometry. After each sub-part has been optimized, the sub-parts are composed to obtain the final design. The case study of a reactor for methanol synthesis supports the results of this paper.

Keywords: Design Automation, Knowledge Based Engineering, Process Engineering, Design for Additive Manufacturing

1. Introduction

The capabilities of modern production methods such as additive manufacturing (AM) allow an increasing complexity of products today. Moreover, fierce global competition increases the demand for innovative complex products and lengthens the product development process considerably [1]. How quickly companies bring innovative products to market plays a crucial role regarding success of the product in the market. Product development plays an active role in the time to market [1]. Companies launch different generations or variants of a product to meet different standards and to keep the product attractive for customers that makes the product tree more complex. However, they also tend to use repetitive design features to simplify the product development and manufacturing process in order to keep the high success rate in qualification tests. Some industries, such as process engineering, have even more repetitive design features due to high qualification standards. According to Stokes [2], 80% of all manual design activities are routine design activities that do not add value to the design. Automation of such routine design activities can be the key to reduce product development time. Although design automation systems are one of the popular topic currently, such systems require high computational resources to provide reasonable results in the presence of multiphysics optimization problems.

The present paper provides an automated system to generate repetitive design features for multiphysics optimization problems where human creativity is not required, thus freeing

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design resources for creative, value-adding tasks. Section 2 describes the state of the art of design automation systems and explains why a new methodology is required for these systems. Section 3 provides the overall workflow as well as the details of each steps in the workflow. The workflow is supported by a case study in section 4. After conducting the case study, conclusions and possible future improvements to the workflow are discussed.

2. State of the Art

Cederfeldt and Elgh [3] define design automation as developing reusable computer functions, which support the design process. There are two main approaches namely computational design synthesis (CDS) and knowledge based engineering (KBE) in design automation [1].

2.1. Computational Design Synthesis

CDS aims to generate design alternatives computationally in the early stages of the design process in accordance with defined requirements. In this manner, optimal structures can be found for the application. One way to generate design alternatives is to use topology optimization (TO). However, the results obtained from the TO should be interpreted and applied by an expert designer because the result may not always be manufacturable or reasonable [5]. Moreover, since the results obtained from TO are non-parametric, this has a negative impact on the next stages of the automation task. Therefore, a parameter based CDS system should be developed to remove user influence from the automation system [5].

2.2. Knowledge Based Engineering

KBE focuses on avoiding repetitive tasks and reducing development time of a design. Repetitive tasks are reduced by incorporating knowledge from previous designs into new designs. KBE has three steps: knowledge capture, formalization and representation [6]. The knowledge capture phase gathers information from proven design concepts to support the design process. The captured information is then organized in a structured way into rules, objects or agents in the KBE system by adding geometric information [6].

Previous works developed valuable methods to identify repetitive design tasks with a KBE system. These methods mostly serve to create a feature taxonomy for large assembly designs [7,8]. However, each part in an assembly can also have features that do not require creativity. The knowledge from these parts should also be captured by KBE systems. In other previous studies, KBE systems were developed for each part and the information captured by the KBE system was used for generating various design variants with different CDS systems that developed for multi-flow nozzles [5] and crankshaft [9], respectively. Such a CDS system with knowledge capture capability improves the feasibility in the market and the accuracy of design automation. However, some products, such as reactors in process engineering, require long multiphysics simulations. In these products, it takes days for a simulation to converge [10]. Automatically building and simulating these products with workflows from previous studies can take weeks of computational time. Therefore, a new optimization system is necessary for the products that need long simulations. This paper addresses this research gap.

3. Methodology

Algorithmic modelling provides high flexibility in design in response to changes. Compared to other modelling techniques such as parametric or direct modelling, logical connections can be established with this technique. This enables users to design not only an object, but also a process [11]. With this kind of understanding, CAD software can evaluate simulation results and optimize geometry with decision-making structures accordingly. The presented paper utilizes this knowledge from the literature and proposes a novel methodology for the product development that require extensive simulations. We illustrate stages of our methodology in Figure 1.

3.1. Knowledge Capturing Mechanism

In a classical product development process, a concept is developed by defining the functions and their structures of the part according to the requirements [12]. Then the design is divided into modules to realize the solution principles. Once all modules are properly designed, the modules are combined to form the complete part [12]. In this process, these modules can be called sub-parts, and the part structure, which is the knowledge of sub-part dependency, can be thought of as the part architecture.

In the first step, we reversed the above workflow to capture knowledge on the part architecture of a proven part concept from the literature. Once this knowledge is captured, the part is decomposed into sub-parts according to the functions in the part architecture. Each sub-part has a single function that is related to other functions, but each of them needs different validations. Besides they should have no conflicting objectives with other functions. At this stage, all sub-parts are listed and prioritized according to the importance of their function. However, there are sometimes conflicting goals between the sub-parts, making them difficult to verify individually. Here, they are considered as a combination of sub-parts and verified together. This boundary definition brings the advantage that optimum sub-parts can be considered also as optimum to the whole part.

The verification is done through simulations which are linked to the algorithmic model to have closed loop automation in the whole optimization process. Suitable types of simulations are selected according to the functions of each sub-part. These simulations can verify structural mechanics, flow properties, other physical properties of the sub-parts or manufacturability. However, in this research we evaluate only the operational performance of the part. Therefore, we assume that the part is manufacturable and focus the verification on functionality.

In this research, we used object-oriented programming to define the part as main object and each sub-part as class. According to an object-oriented programming, every class has functions and attributes. Attributes refer to information of the

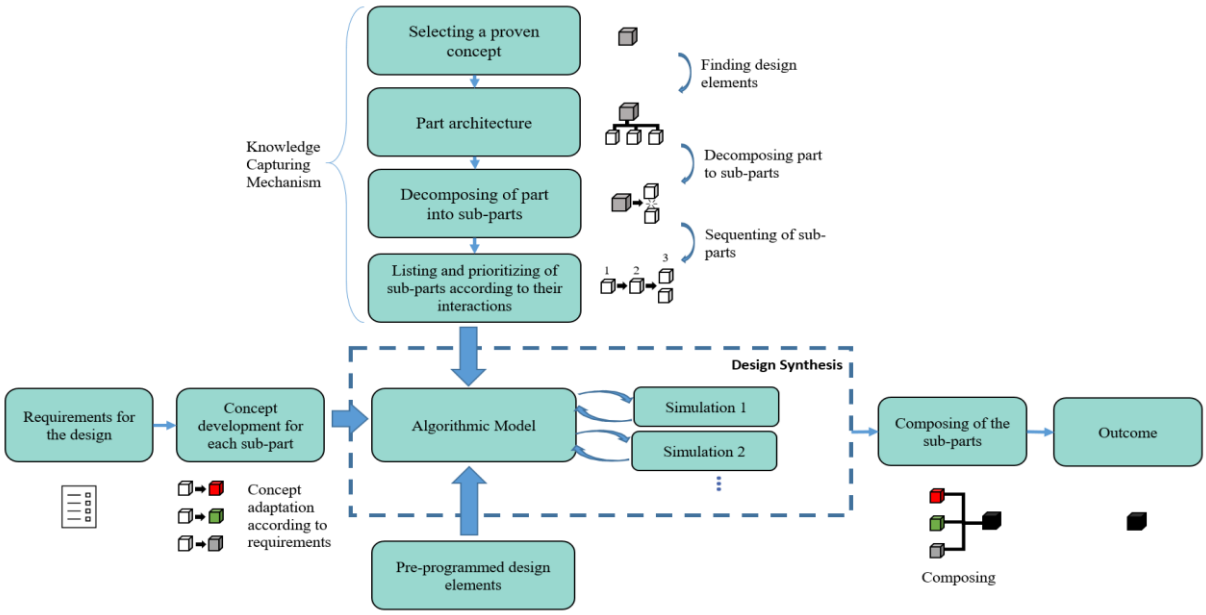

Figure 1: Design automation workflow for products that need long simulations

classes. Functions can modify or update the object [13]. Every sub-part has the knowledge to modify the part through its function and to make decisions through its attributes on which simulations are done to verify the structure of the sub-part. A case study demonstrates this method in section 4.

3.2. Design Synthesis

The captured information is used to define the algorithmic model. However, firstly the requirements are investigated to synthesize the information obtained in the design. The performance of a design is directly related to the concept idea. Also, creativity is required in the concept phase. Therefore, only this phase is done manually by the designer. In this step, manufacturing constraints are also taken into account, since there is no automatic control mechanism in the workflow due to the additional requirement of computational resource as described in Section 3.1. Once the concept is developed, an algorithmic model is created in a 3D-CAD software such as *Rhinoceros*® or *Siemens NX* using pre-programmed design elements from an available database. The database is used to increase the number of variants of each sub-part [5].

In the classical development workflow, a non-detailed solid model is first created to optimize the structure of the part. Then the part is simulated according to the requirements and in each iteration of the optimization the part is redesigned according to the results obtained from the simulation or optimization software.

The method proposed in this paper integrates and synthesizes the classical product development steps. According to our method, not only the 3D model is developed in CAD software, but also the development process. First, possible simplifications for each sub-part simulations are investigated. Furthermore, it is examined which parameters have an impact on the simulation results. If more than one simulation is required to verify the sub-part, the simulations are sequenced in a logical order to reach the optimal sub-part in the fastest way. After this decision, the input geometries for the first simulation are designed and the simulation software is connected to the CAD software by using an automation software. To automate the connection of CAD and simulation software, only one simulation is prepared manually in order to define physics correctly. After that, the input geometry is imported to the simulation software in every iteration and the simulation is executed automatically. Using logical decision-making structures in the CAD software, a small loop is created to optimize based on the simulation result. Parameters that have a high impact on the simulation results are optimized in this loop. After a first optimization loop, the optimized structure is used to build an input geometry for the next simulation task. This process is done sequentially for all simulations. Hence, it is possible to optimize geometries in local loops through an algorithmic model. This approach reduces the required amount of computational power because the whole model does not have to be recalculated for each parameter changes.

Once the sub-part is optimized, the design synthesis process is applied for all sub-parts. As mentioned earlier, each sub-part needs different verifications. With this methodology, simulations for verifications are only done locally within the part. In addition, the methodology allows to optimize different variants of the sub-parts automatically. Once the verification process is complete, all the sub-parts are merged with each other, and the part is created. The part is optimized and verified consequently. For regulatory reasons, the design still needs to be validated at the system level before it can be operated.

4. Case Study

In this section, a case study is presented to demonstrate the effectiveness of the proposed design automation methodology for products that require long simulations. One example of such products are reactors in chemical process engineering. Various types of reactors are widely used in different sectors such as the pharmaceutical or energy industry. Different requirements are essential to design a successful reactor for each application. The validation of each reactor design requires detailed reaction

simulations because a reactor design is a complex multiphysics problem with variable material parameters. In addition, an optimum reactor design depends on many different input parameters such as volumetric flow rate, concentration, temperature, pressure, and catalyst volume. This increases the need for a high number of optimization cycles. Therefore, the reactor design is chosen for the application of the proposed methodology. In this research, we used the developed design automation system to design a reactor for methanol synthesis.

Methanol (CH_3OOH) is a chemical intermediate widely used to produce alternative fuels such as dimethyl ether (DME) or to store electricity from renewable sources such as wind or solar energies. Its synthesis is an exothermic reaction, a cooling system is required to maintain the operation temperature in the methanol reactor within an acceptable range. As an example, multitubular packed bed reactors can be operated at high pressure (50-80 bar) and relatively high temperatures (200-300°C) on an industrial scale for methanol synthesis [14]. Due to the high-pressure operation of methanol reactors and the high safety regulations for acceptance according to DIN EN 13445 norm, reactors need to be validated by an extensive testing or simulation program. In addition, the wall thickness of the channels of the methanol reactor should be as thin as possible to increase heat transfer. This challenge in methanol reactor design increases the necessity of testing not only from a structural point of view but also from a chemical aspect.

The required test process for an acceptance and restrictions of traditional manufacturing methods limits the number of different reactor types. These classical reactor types such as multitubular packed-bed reactors are well-known, proven systems in the industry. Therefore, analytical solutions are developed for the dimensioning of the reactor. However, with technological advances in production systems such as AM, complex methanol reactors can be produced. As a consequence of this progress, analytical solutions are not sufficient to optimize a methanol reactor and numerical solutions are needed. However, for the simulation of the part according to DIN EN 13445 annex B, the entire part must be simulated together. Therefore, only the structure that affects the heat transfer phenomenon should be optimized in an optimization cycle. The external structure can be optimized in the system level. In order to reduce the computational resources required for reactor optimization, the methodology proposed in this paper is implemented as follows.

4.1. Knowledge Capturing from Proven Concept

To understand the part architecture of methanol reactors, a multitubular packed-bed reactor is selected as a proven concept. The classical multitubular packed bed reactor has 2 inlets and 2 outlets. In the operation of the reactor, reactants enter through the first inlet. Reactants are raw materials in chemistry. In the case of methanol synthesis, carbon dioxide (CO_2) and hydrogen (H_2) are the reactants and an inert gas such as nitrogen (N_2) is also used to avoid unwanted chemical reactions. In some cases, carbon monoxide (CO) is also used to produce methanol. The reactants react with each other using catalyst until an equilibrium of the reaction is reached. Products and remaining reactants leave the reactor as through the outlet.

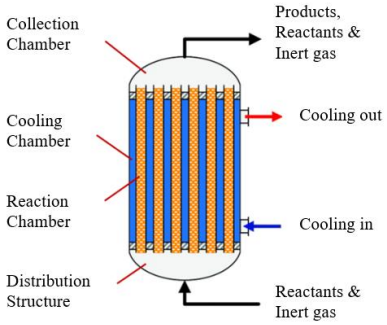

Figure 2: Multitubular packed-bed reactor adapted from [15]

The reaction is exothermic and releases heat, therefore the reactor is cooled by a cross-sectional and countercurrent flow system through a second inlet and outlet.

Figure 2 depicts this type of reactor as an arrangement of four sub-parts. The first sub-part *"Distribution Structure"* has the single function of evenly distributing the mixed gas flow in the channels. There is no catalyst in this sub-part, so no reaction takes place. For verification, this sub-part only needs to be simulated to optimize the flow properties and there is no need for a complex reaction simulation. Moreover, since there is no heat transfer phenomenon in this sub-part, there is no need to optimize the sub-part in terms of structural mechanics as mentioned above.

Once the reactants reach the catalyst particles in the tubular channels, the reaction takes place with an interaction between reactants and catalyst. These tubular channels can be named as *"Reaction chamber"*. Due to the importance of the surface mechanism of the catalyst and the heat transfer properties of the channel structure, complex reaction simulations should be performed on this sub-part. With these simulations, the flow and heat transfer properties of the geometry of the sub-part are studied. However, these simulations cannot be performed without knowing the cooling behavior in the reactor system. Therefore, the *"Cooling Chamber"* cannot be considered separately from *"Reaction chamber"*. In addition, the structure of the channels must be optimized in structure mechanics aspect. However, these structures, especially the wall thickness of the channels affect the heat transfer as well as the mechanical integrity. Therefore, they cannot be optimized afterwards like *"Distribution Structure",* and they must be taken in optimization loop. Therefore, multiple simulations are required for the *"Reaction chamber"* and *"Cooling Chamber"* sub-parts.

After the reaction has taken place and the products and residual reactants leave the channels. They are collected in the *"Collection chamber"* and leave the whole reactor through the outlet. This sub-part has no other function than to collect all products and reactants. Therefore, there is no need for a simulation for the flow characteristic. Only the external structure must withstand the pressure in the reactor and the designer must consider the pressure drop.

Table 1 lists the sub-parts and prioritizes them according to their importance for the reactor. The most important function in a methanol reactor is the conversion of methanol and it is determined in the *"Reaction chamber"*. The *"Cooling chamber"* has also same importance because it cannot be optimized separately, as described above. After this optimization loop, the *"Distribution Structure"* is optimized

because its function is more important than *"Collection chamber"*. The interface geometries from *"Reaction chamber"* are considered in the optimization of the *"Distribution Structure"* and the *"Collection chamber"*. The computational design synthesis of the sub-parts is done in this order.

Table 1. The sub-parts and required simulations for a verification

Sub-Parts	Importance	Required Simulations	Objective Function	Constraints
Reaction and Cooling Chamber	1	Complex CFD	Maximize Conversion (U)	$220°C < T_{in} > 280°C$ $\Delta p < 10$ bar
	1	FEA	Minimize Wall Thickness (d)	Stress (σ) < 237,5 MPa Strain (ε) < 5%
Distribution Structure	2	Simple CFD	Minimize Flow-Maldistribution	-
Collection Chamber	3	-	-	-

4.2. Design Synthesis of Methanol Reactor

The design synthesis and optimization workflow is implemented in *Siemens HEEDS*. The software is used to open and connect CAD and the simulation software, as shown in Figure 3. This makes the optimization of structure parameters a closed loop. In this loop, when to run the simulation is determined in the CAD software through algorithmic modeling.

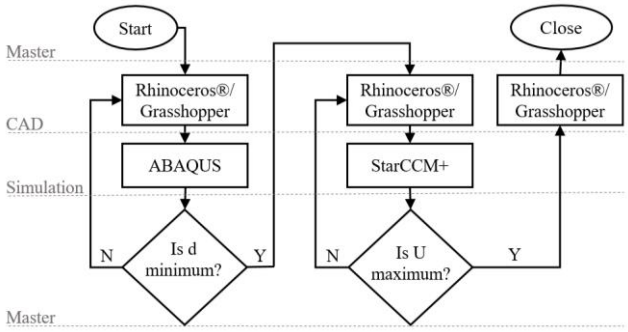

Figure 3: Used algorithm from HEEDS for optimization of the "Reaction Chamber"

Algorithmic modelling makes it possible to build decision-making structures in CAD software. With such structures, different parametric optimization cycles can be defined in a single CAD model. To optimize the *"Reaction chamber"* first, an algorithmic model is created using the *Grasshopper* plug-in of *Rhinoceros*® software. A parametric model is created in *Grasshopper* to define the geometry of the sub-part mathematically. The number of the variants for the sub-part *"Reaction Chamber"* is increased by using pre-programmed design elements, as demonstrated for multi-flow nozzles by Biedermann et. al [5]. Production constraints are considered in the modeling and the concept is developed with this information. Other requirements of the methanol reactor are also taken into account and the objective functions and constraints are defined for the necessary simulations as shown in Table 1.

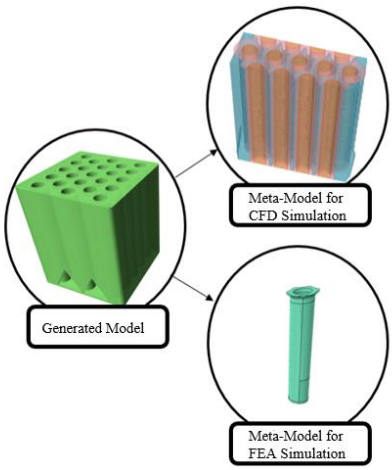

Figure 4: Meta-models for the simulations in the "Reaction Chamber"

Due to the requirement of multiple simulation types as shown in Table 1, two simulation loops are created in the model. A pseudo-static model is created in the *ABAQUS* software to simulate the behavior of the structure in the first loop (see Figure 3). The pressure inside of the channels from the reactants and the pressure outside due to the coolant are considered as the loads in the system. Since the whole chamber consists of the equal channels, the model can be simplified and only one channel can be taken as a meta-model for the further simulation phase (see Figure 4). A meta-model is an inexpensive deterministic approximation function for the calculation of the quality criteria of the simulation [16]. The decision-making structure in *Grasshopper*, avoids the need to calculate the whole CAD model for parameter optimization. Until the end of the first optimization loop, the other features are frozen by the *Metahopper* plug-in.

Once the parameters are optimized for mechanical requirements, *HEEDS* starts another simulation loop on a CAD model representing the thermal management components (see Figure 3). This loop uses *Starccm+* as a CFD software to simulate methanol synthesis. In order to define the reaction kinetics, the common model from Vandan Bussche et. al. [17] is used. Furthermore, the initial conditions for the reaction and the type of the catalysis are considered as the same in the reaction's kinetic in Vandan Bussche et. al. With using conjugate heat transfer mechanism from *Starccm+*, the interaction between *"Reaction Chamber"* and *"Cooling Chamber"* is simulated. Because of the symmetry in the model, a meta-model of the geometry is created, as shown in Figure 4. After the second optimization loop, the sub-part is created. The whole optimization process for *"Reaction Chamber"* took only 50 minutes, which shows the computational advantages of the method over classical optimization. However, the required computational time can increase with usage of more complex design elements. To avoid unnecessary repetitive calculations in *Grasshopper* during the automation process, the same freezing features idea of the *Metahopper* plug-in is used, as described above.

As an advantage of the proposed methodology, the other sub-parts are not simulated with complex reaction definition. The sub-part *"Distribution Structure"* is created with the results from the sub-part *"Reaction Chamber"* such as the positions of the channels and their diameters. In this sub-part,

the geometry is only optimized to distribute the reactants in the channels equally. On the other hand, the last sub-part *"Collection Chamber"* is created with using the knowledge from the sub-part *"Reaction Chamber"*.

After all sub-parts have been optimized, they are combined with each other in *Grasshopper*. Thus, a new design is created using the proposed methodology. The number of variants of the reactor is increased by changing the design elements in the database. The design and simulation steps are embedded in *HEEDS* software to automate the whole process.

5. Discussion

This work introduces a digital workflow for the creation of an automated design for products that need lengthy simulations for verification. The workflow shows how the part is divided into sub-parts and what verifications are required for each sub-part. The knowledge capturing mechanism helps the designer to organize the requirements for each sub-part individually. In addition, this method greatly reduces the use of computational resources by verifying all sub-parts separately. This separation allows dedicated simplifications of the sub-part geometry for each simulation. This method enables not only to reduce the computational time, but also to create an integrated product development method.

Currently, we use pre-programmed design elements to increase the number of design variants. In terms of design and production, the workflow works flawlessly. However, it has the following limitations:

- Although using the database is increasing the number of the variants, it increases also the required computational time, because the workflow must be recalculated for each variant.
- Due to the verification of all sub-parts individually, it is difficult to validate the workflow experimentally. A basic experimental validation structure is required.
- Because of the complexity of multiphysics problems, pre-programmed design elements are used in this method only in the same part architecture. However, the method can be further improved using the function integration advantage of AM.

The next step is overcoming these limitations and experimentally validate the workflow. Further, the workflow will be adapted for the different tasks and applications.

6. Conclusion

In this paper, a digital integrated product development workflow is presented for the automatic generation of the algorithm-based designs. Starting with a knowledge capturing mechanism from a proven concept to find the part architecture and then decomposing the part into sub-parts, an algorithmic model is defined for each sub-part. In the algorithmic model, the sub-parts are optimized dynamically with different simulation in an integrated way. The digital workflow is supported with a case study of the reactor design for the methanol synthesis. After demonstrating a case study, the results are discussed and possible further improvements in the workflow is shown.

Acknowledgements

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