A Graph Database Approach for Supporting Knowledge-Driven and Simulation-Based Optimization in Industry and Academia

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Abstract. With the increase in complexity of industrial systems it becomes more and more challenging to make well-grounded decisions for system design and operation. Following the concept of Virtual Factories with Knowledge-Driven Optimization (VF-KDO), this paper proposes a graph database approach to support knowledge-driven and simulation-based optimization. With the mapping of a VF-KDO ontology to a graph database, competency questions that facilitate traceability, transparency, and group decision making can be answered. This is exemplified with an industrial use case and different student projects from an education course in Industrial Engineering and Management.

Introduction

With the advent of Industry 4.0, industrial systems are becoming increasingly complex, interconnected, and reliant on digital technologies. The amount of heterogeneous data produced by sensors, machines, and automation tools is growing exponentially. This complexity presents a major challenge in terms of data integration, knowledge extraction, and decision-making. In terms of decision-making, in modern industrial settings, optimization and simulation-based decision-making play a crucial role in enhancing operational efficiency. Virtual manufacturing, simulation, and optimization processes generate a wealth of knowledge. However, much of this knowledge remains siloed, accessible only to domain experts, and difficult to share or reuse effectively. The need for an integrated and systematic approach to storing, managing and re-using such knowledge has never been more pressing.

To address these challenges, the concept of Virtual Factories with Knowledge-Driven Optimization (VF-KDO) has emerged as a novel approach to enhance optimization potential in factory design and operation. The core idea behind VF-KDO is to leverage the uses of Simulation-Based Optimization (SBO), particularly Multi-/Many-Objective Optimization (MOO), running on virtual factory models and then use advanced machine learning to extract knowledge and identify patterns from the optimized outcomes in order to derive higher-level insights. MOO is particularly important to such a VF-KDO concept when observing that existing optimization methods usually fail to adequately capture relationships between decision variables and multiple conflicting objectives.

Furthermore, many Decision Support Systems (DSS) assume a limited set of predefined solutions, neglecting the rich connections between historical optimization experiments or decision-support scenarios with the ongoing decision-making processes.

This paper proposes a graph-database-driven approach to support SBO in general and Knowledge-Driven Optimization (KDO) in specific by leveraging Knowledge Graphs (KGs). Specifically, by mapping a VF-KDO ontology into a graph database implemented in Neo4j, we aim to facilitate traceability and transparency, as well as support group decision-making and analyses in both industrial and academic research and educational environments, as exemplified in this paper.

The remaining sections of the paper are organized as follows. Section 1 presents a literature review to justify the research gaps that we aim to address.

Section 2 briefly introduces the VF-KDO methodology and its ontology, which underpin this line of research. Sections 3 and 4 present the proposed graph database approach and its implementation using Neo4j, respectively. Industrial and academic use cases, along with their evaluations, are covered in Section 5. Finally, Section 6 concludes the paper and outlines future work.

1 Literature Review

While prior research has explored the application of KGs and semantic web technologies in industrial optimization, significant gaps remain. Existing studies have primarily focused on the following areas:

1.1 Graph Models for Decision Support

Graph-based knowledge representations have emerged as a powerful paradigm for DSSs, offering advantages that traditional relational databases struggle to provide. Elnagar and Weistroffer [1] argue that KGs offer several key benefits for decision support, including scalability, timeliness, ease of data integration, and interpretability for both human and machine users. They envision KGs as the central collector of all knowledge sources upon which data models are built and inference tasks executed. However, they also acknowledge challenges such as maintenance of large KGs, comparison of different graphs, and the fundamental issue of data quality, which impacts any subsequent task.

Within the specific domain of multi-objective optimization, several DSSs have been proposed. Li et al. [2] developed a system that combines self-organizing maps with data envelopment analysis to help decision makers identify the most suitable solution on the Pareto front of a multi-objective optimization problem. For group decision-making contexts, Rosanty et al. [3] demonstrated how social choice methods can extend the Analytic Hierarchy Process to function effectively for group decisions. More recently, Li et al. [4] proposed a framework to address the heterogeneous nature of preference expressions, which represents one of the key difficulties in group decision making.

Smedberg and Bandaru [5] presented a DSS specifically designed for interactive knowledge discovery during Pareto front exploration. Their approach allows decision makers to investigate the relationship between variable space and objective space, facilitating deeper understanding of the problem and the potential implementation impacts of different solutions.

Zheng and Wang [6] reviewed recommender systems that aim to yield recommendations with respect to multiple objectives, noting that group fairness becomes an additional objective in collective decision contexts, and highlighting the persistent challenge of making recommendations in the absence of explicit preferences.

1.2 Graph-Based Industrial Applications

KGs have found many practical applications across a range of industrial contexts, particularly in manufacturing systems. Hoppen et al. [7] described a procedure to map and synchronize KGs in Neo4j with the object-oriented in-memory database of simulation software, enabling persistent storage of simulation model hierarchies. Tang et al. [8] utilized KGs in RDF format to improve power equipment management, focusing particularly on the integration of information from heterogeneous sources including both semi-structured and unstructured information.

In the domain of quality management, Wang et al. [9] developed an ontology-based KG to provide decision support for manufacturing processes. Their human-cyber-physical approach integrates knowledge across multiple levels of the production system. Zhou et al. [10] proposed methods to generate KGs from unstructured information and provide decision assistance through question answering, a capability particularly relevant for industrial processes where documentation exists in natural language forms.

Xiao et al. [11] conducted a comprehensive review of KG applications for manufacturing process planning, concluding that these approaches offer significant advantages over conventional process planning techniques. For discrete event simulation management, Listl et al. [12] proposed a KG-based framework and demonstrated its utility for automatic simulation model generation. Mo et al. [13] used KGs to support reconfigurable manufacturing systems, showing that different typical optimization problems for such systems can be facilitated with recommendations derived from the KG.

Zhou et al. [14] applied ontology-backed KGs to optimize resource allocation in discrete manufacturing workshops. For document management within industrial organizations, Weber et al. [15] built KGs from documents to facilitate retrieval of relevant information, effectively adding context to Industry 4.0 analytics through a new document-driven KG construction and contextualization approach.

1.3 Ontologies for Manufacturing Systems

Recent literature provides comprehensive coverage of ontologies in the manufacturing domain. Sapel et al. [16] conducted a systematic review identifying 65 ontologies, which they categorized according to covered topics. Most of these ontologies focus on resources, processes, and products, while scheduling, maintenance, and sensor topics also appear frequently. Notably, only six ontologies address the simulation domain, and optimization as a topic was not discovered in any of the ontologies reviewed.

Alkahtani et al. [17] utilized the MASON ontology [18] in their DSS to link design data with warranty data. Their system connects component functions from design data with failure reports from warranty data, enabling identification of components causing specific failures and facilitating product design improvements. This represents one of the few examples where an ontology explicitly supports optimization-related decision making in manufacturing. The review by Xiao et al. [11] also examined ontology-based approaches for manufacturing process planning, concluding that KG and ontology techniques can be advantageous over common process planning techniques, though they note that the integration challenges remain.

1.4 Ontologies for Optimization Workflows

The intersection of ontologies with optimization workflows remains notably underdeveloped. Sapel et al. [16] found no ontologies in the manufacturing domain that include concepts relevant for optimization. When extending the search beyond manufacturing, several ontology repositories have been found in our systematic investigation. Particularly, among them, seven ontologies are found to provide some concepts relevant for optimization, including Algorithm Metadata Vocabulary (AMV) [19], Kinetic Simulation Algorithm Ontology (KiSAO) [20], NCI Thesaurus OBO Edition (NCIT) [21], Ontology for Biomedical Investigations (OBI) [22], Ontology of Core Data Mining Entities (OntoDM) [23], Ontology for Simulation, Modelling, and Optimization (OSMO) [24], and Physicalistic Interpretation of Modelling & Simulation: Interoperability Infrastructure (PIMS-II) [25]. Among these, KiSAO and PIMS-II include simulation concepts, but none is targeted at manufacturing optimization. The evaluation of these ontologies against six ontologies with simulation concepts identified by Sapel et al. [16] reveals a significant gap: no existing ontology adequately captures the concepts and relationships essential for knowledge-driven optimization workflows, including optimization algorithms, solution sets, Pareto frontiers, decision rules, and the connections between these entities and simulation models.

Maciol et al. [26] claimed to describe an ontology for KDO, but upon closer investigation, only a small subset of the ontology was presented in the paper without the link to a full ontology. The presented subset suggested little to no terms directly relevant for knowledge-driven optimization as defined in the present work. Instead, their ontology appears to be aimed at reasoning within optimization projects to obtain knowledge that can improve the optimization approach itself aimed by the conception of KDO. The need to manage provenance for optimization is recognized [27] and graph databases are a suitable tool for that [28]. However, the traceability from simulation model over optimization runs to preferences and decision is often neglected.

2 VF-KDO Methodology & Ontology

The approach proposed in this paper builds on the prior efforts related to the VF-KDO methodology and its algorithms [5, 29], but specifically introduces a graph database implementation of a VF-KDO ontology, ensuring seamless integration of optimization, simulation, and decision support in an accessible and queryable format. Unlike pure ontology-driven approaches, our method takes advantage of graph database capabilities, such as fast traversal, relationship-based queries, and real-time knowledge updates.

On the other hand, unlike the specific architecture described by Listl et al. [12] that focuses on integrating KGs into simulation environments to support "endogenous" simulation project life cycles, our work aims at a cutting-edge exploration of how an integration of simulation, MOO and machine learning will shape future knowledge-based decision-support systems that effectively store and re-use the generated "exogenous" simulation and SBO knowledge.

The VF-KDO Ontology, schematically illustrated as a class hierarchy diagram in Figure 1, provides a structured vocabulary for representing artifacts and their relationships within the VF-KDO methodology, organized to support traceability and reusability across optimization projects.

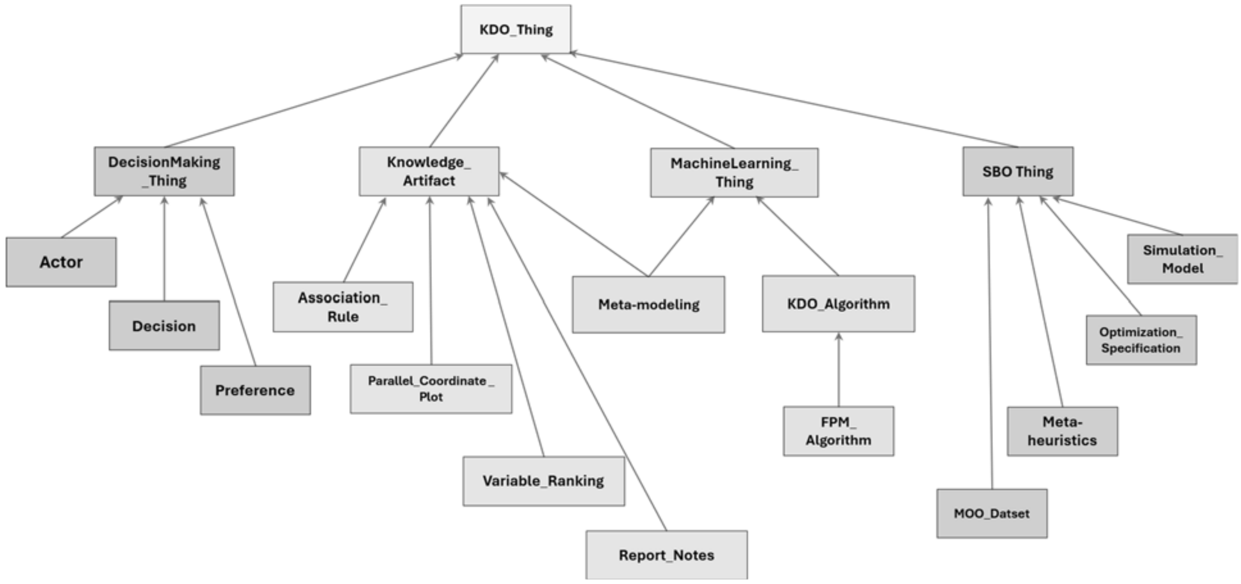

Figure 1: High-level class hierarchy of the VF-KDO Ontology.

At the root is *KDO_Thing*, from which all entities represented within the VF-KDO framework and data saved in the graph database implementation are inherited. A unique relationship observable from the VF-KDO Ontology is the *Knowledge_Artifact* as a special subclass of KDO_Thing captures any product of knowledge generation through the *MachineLearning_Thing* (models, algorithms, and pattern discovery techniques). Under *MachineLearning_Thing*, *KDO_Algorithm*, such as the *FPM_Algorithm* [29] captures algorithm-specific configurations for generating *Association_Rule* and *Variable_Ranking* as subclasses of *Knowledge_Artifact*. *MOO_Dataset*, generated through running *Meta-heuristics* on *Simulation_Model* using the problem formulation (objectives, decision variables and constraints) and algorithm settings defined in the *Optimization_Specification* captures MOO solution sets and Pareto frontiers.

Under *DecisionMaking_Thing*, *Decision* captures actual stakeholder choices, *Preference* represents expressed objective priorities and constraints articulated by decision maker(s). Such a VF-KDO Ontology serves as the backbone of the KG connecting simulation models, optimization runs, solution sets, discovered rules/patterns, and decisions. Instantiating these classes enables traceability from decisions to specific results and models, reusability of knowledge across projects, interoperability across software tools and domains (e.g., logistics and robotics), and cumulative learning as the growing graph reveals cross-case patterns and transferable principles.

3 Graph Database Approach for KDO

At the core of the proposed approach is a graph database structure that maps the VF-KDO ontology to a property graph model (see Table 1). By storing simulation models, optimization variables, objectives, and Pareto-front solutions as graph entities, it enables quick retrieval of relevant optimization runs based on similar decision-making scenarios or various design experiments historically conducted in a company or within an academic institution.

Apart from enabling any cross-referencing between past simulations, optimization and extracted knowledge with real-world data, this approach can also facilitate deriving new insights for supporting new decision-making. In terms of group decision-making, this approach can enable traceable and transparent decision support as it links decision variables to stakeholder preferences and previous decisions which in turn make it possible to allow further decision process analysis to uncover biases and inconsistencies.

With a DSS system developed atop of such a graph database, it will provide visualization and query mechanisms for stakeholders to collaboratively explore solutions as well as integrate feedback loops where past decisions inform future optimizations. The latter can be achieved by using machine learning based heuristics to suggest optimal decision paths from numerous SBO/KDO scenarios stored in the graph database.

Ontology element	LPG element
Class	Node
Object Property	Node
Annotation	Node Property
Subclass Axiom/Restriction	Arc
Restriction Quantifier	Arc Property

Table 1: Mapping between ontology and LPG elements.

More advanced machine learning algorithms, e.g., like graph-based clustering and pathfinding, can be further developed to extract patterns from historical optimization data and trace back these patterns through graph-based queries to gain higher-level and generalized principles for organization within a company and/or student learning in an academic setting.

While most relations in the ontology are kept simple, the inclusion of production principles requires some clarification. Production principles follow the structure condition implies consequence, where both condition and consequence can consist of several logical connected parts. Hence, the structure in Figure 2 follows. As a basis for the more advanced functions mentioned before, competency questions are formulated to guide ontology construction and query creation.

Examples for competency questions regarding optimizations are:

- What are the objectives for this optimization?
- What are the variables involved in this optimization?
- Which optimization algorithms were used for all the optimizations performed on this model?

For the academic scenario, questions related to production principles and the associated variables and performance measures are interesting:

- Which studies are related to principles about this variable?
- Which studies are related to this performance measure?
- Which principles link this variable and this performance measure?

4 Implementation Details

The graph database of our choice is Neo4j, because of its support for the labelled property graph model and its popularity in industry. Neo4j provides the Cypher query language to interact with the data. Therefore, the first step to integrate the ontology in the graph database is to create Cypher statements that create nodes and edges according to the ontology. To do this programmatically, we used Python and the Neo4j Python driver.

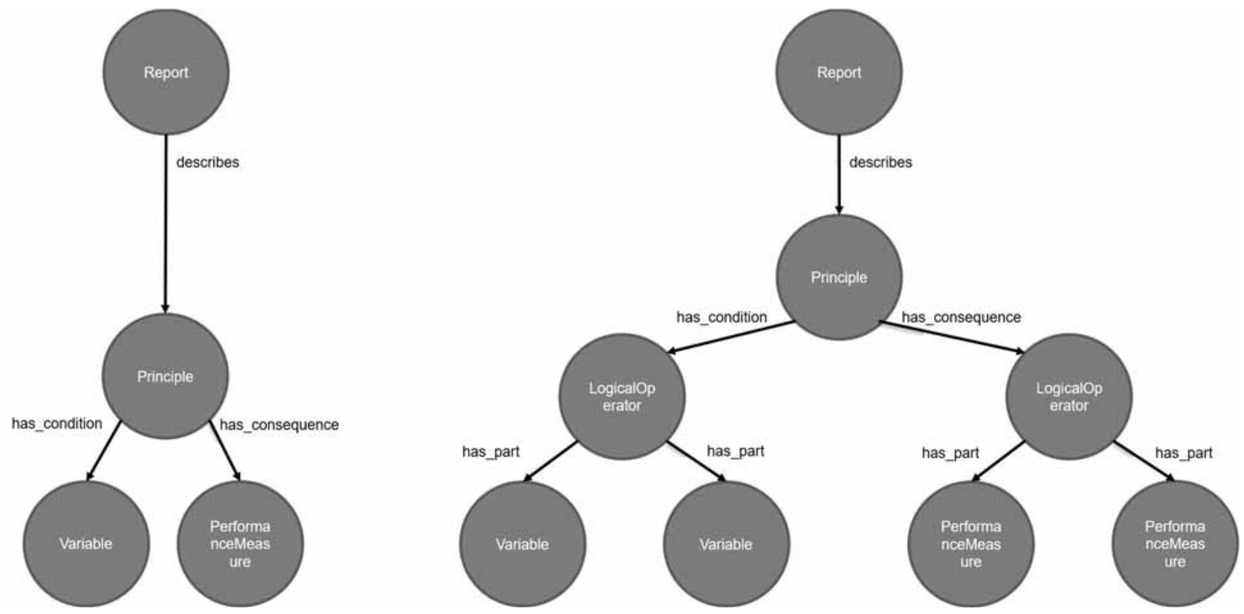

Figure 2: The structure for principles in the case of one variable and one performance measure (left) and in the case of multiple variables and multiple performance measures connected via a logical operator (right).

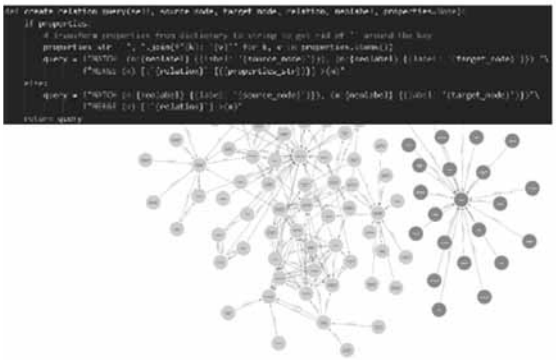

Figure 3: The ontology for knowledge-driven optimization after import through Python scripts (example in black box) in the GDB with classes in yellow and object properties in blue.

The ontology was developed in Protégé and not directly in Neo4j, because of the simpler editing. For the same reason, a script was created that exports the ontology back to owl. However, it is possible to include new concepts in the ontology directly in the graph database. This is particularly useful for project specific data that is not universal for all KDO projects. Figure 3 shows the ontology in the Graph Database (GDB) along with a snippet from the Python code that generates the Cypher queries to import the ontology to the GDB.

5 Use Cases and their Evaluations

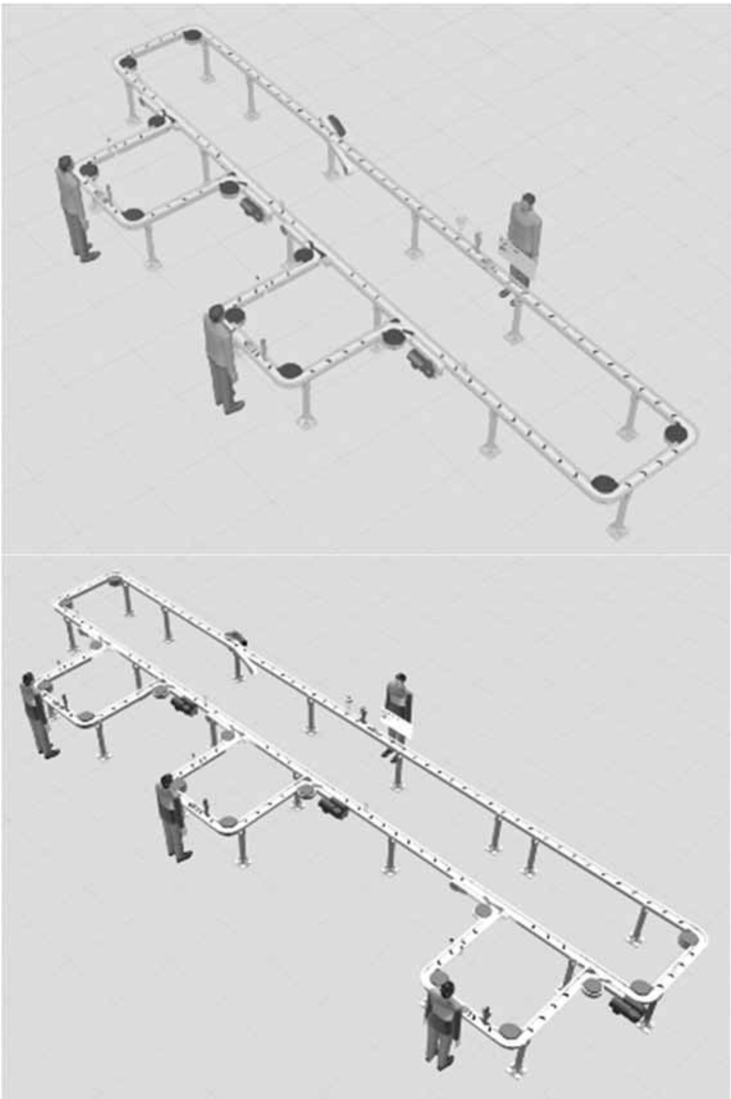

Figure 4: The two simulation models from the industrial use case: one with two satellite conveyors (top) and one with three (bottom).

Two use cases, one from industry and one from academia, demonstrate the usefulness of the GDB. The industrial use case is based on a cooperation with FlexLink AB. Two simulation models of two slightly different conveyor systems are used to optimize the respective system with respect to throughput and a cost function. In the academic example, students created simulation models to study production principles. With the GDB, it becomes easy to answer questions about these use cases.

5.1 Industrial Use Case

The first simulation model from the industrial use case comprises a main conveyor with two satellite conveyors where at each of the conveyors is a workstation (see Figure 4). The decision variables are the speeds of each of the conveyors (MainSpeed, SatSpeed1, SatSpeed2) and the number of pallets.

The resulting objectives for the optimization of this model are to maximize throughput and minimize a cost function:

- Maximize Throughput
- Minimize Cost = (MainSpeed +
  + SatSpeed1 + SatSpeed2)/100 +
  + NbrOfPallets

The second simulation model is almost identical to the first one (see Figure 4), but with one additional satellite conveyor and hence one more decision variable (Sat Speed3).

This is also reflected in the cost function for the optimization objectives:

- Maximize Throughput
- Minimize Cost = (MainSpeed + SatSpeed1 + SatSpeed2 + +SatSpeed3)/100 + NbrOfPallets

The available information about these optimizations was added to the GDB according to the ontological structure. Now, if someone wants to know with which algorithm the optimizations of the models were done, it is relatively simple by executing the query shown in Algorithm 1. It reveals that in this use case, both optimizations were done with the NSGA-III algorithm (see Figure 5).

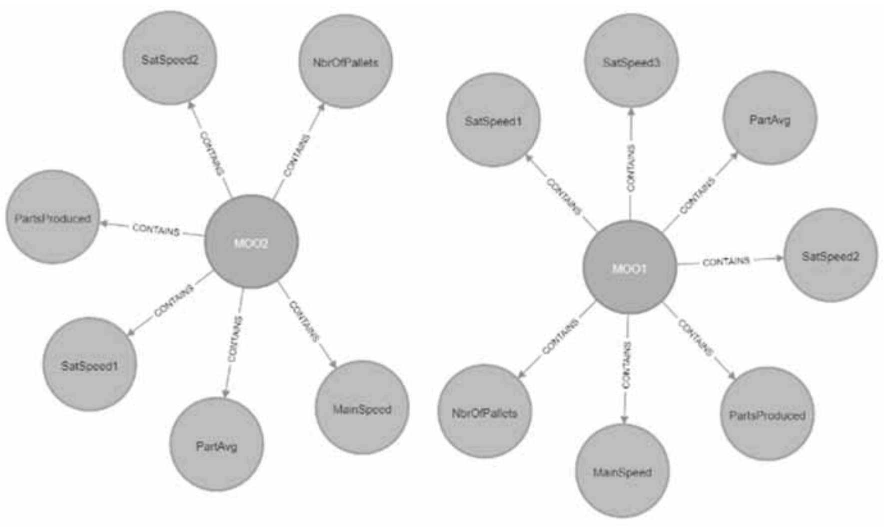

Figure 6: Visualization of the query result, which shows the variables (green) that are a part of each of the optimizations (orange).

Algorithm 1: Query to retrieve the optimization algorithm used for the optimization of each of the models.

```
MATCH (n:Model)-[:DEFINES]->
(m:OptimizationFormulation)-[:SETS]-
>(0:KDOAlgorithm)
RETURN n, m, o
```

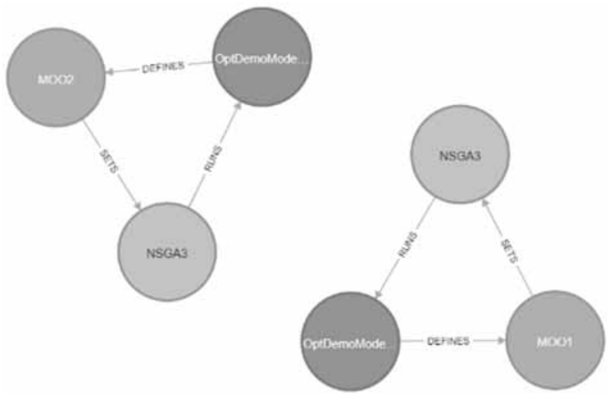

Figure 5: Visualization of the query result, which shows the algorithm (pink) used for the optimization (orange) of each of the models (red).

Another interesting information is which variables are considered in the model. The query in Algorithm 2 retrieves the variables for each model (see Figure 6). Alternatively, the query in Algorithm 3 reveals variables that are used in one model only (see Figure 7).

Algorithm 2: Query to retrieve the variables involved or affected by each of the optimizations.

```
MATCH (n:OptimizationFormulation)-
[:CONTAINS]->(m:Variable)
RETURN n, m
```

Algorithm 3: Query to retrieve variables unique to each optimization.

```
MATCH (n:OptimizationFormulation)-
[:CONTAINS]->(m:Variable)
WITH m.name AS variableName, COUNT(m) as
occurrence
WHERE occurrence = 1
MATCH (n:OptimizationFormulation)-
[:CONTAINS]->(m:Variable {name: variable-
Name})
RETURN n, m
```

Figure 7: Visualization of the query result, which shows the variables (green) unique to a specific optimization (orange).

Despite the lack of information about decision makers and their preferences, this use case demonstrates already the value of gathering insights about simulation models and comparing their setup.

5.2 Academic Use Case

The academic use case revolves around student projects within a simulation course in which the students are tasked to build models for the examination of production principles.

From the models, created in FACTS Analyzer, the objectives and variables are imported. These are linked to the model, the report of the students, and the principles that were examined in the report. This allows anyone who wants to learn about these principles to find reports and models that are about a particular principle. Furthermore, the students can find principles that relate to a specific variable or performance measure, thus easily deepening their knowledge on the topic.

A student, who wants to find all reports related to WIP as a performance measure, can use Algorithm 4 to achieve this (see Figure 8). With Algorithm 5, a student can find all principles that link the variable "changeovers" to the performance measure "throughput" as shown in Figure 9.

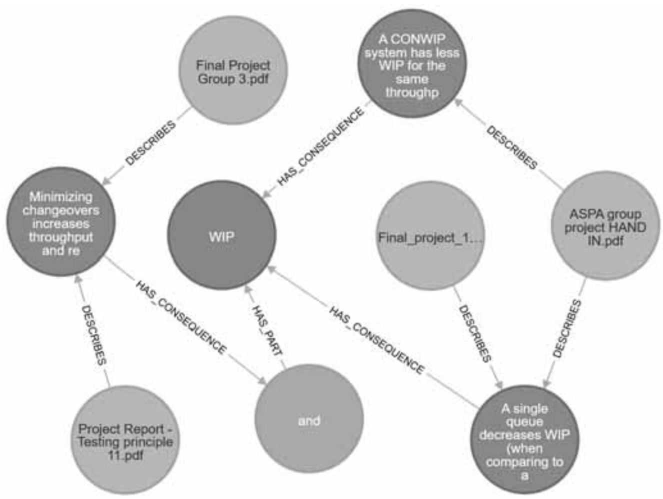

Figure 8: Visualization of the query result, which shows the reports (light blue) that describe a principle (dark blue) that has influence on the performance measure "WIP".

Algorithm 4: Query to retrieve all reports that describe a principle with "WIP" as performance measure.

```
MATCH pp=(v:PerformanceMeasure
{name:"WIP"})<-[*]-(p:Principle)<--
(r:Report)
RETURN pp
```

Algorithm 5: Query to retrieve all principles that link the performance measure "throughput" to the variable "changeovers".

```
MATCH pp=(v:PerformanceMeasure
{name:"throughput"})<-[*]-(p:Principle)--
>(r:Variable {name:"changeovers"})
RETURN pp
```

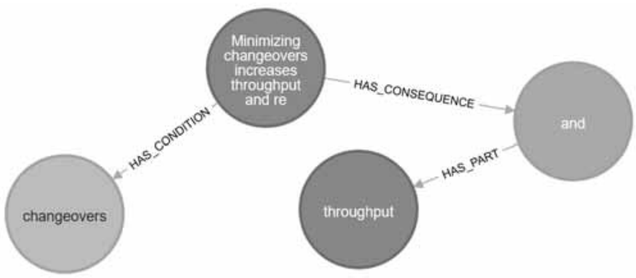

Figure 9: Visualization of the query result, which shows the principles (blue) that link the performance measure "throughput" (dark green) and the variable "changeovers" (light green).

6 Conclusion and Future Work

This paper introduces a graph database-driven system designed to enhance KDO and simulation-based decision support in both industry and academia.

By mapping a KDO ontology to a graph database, the system enables:

1. A structured and queryable knowledge repository for optimization results, including optimal solution datasets and the knowledge extracted from them.
2. Improved traceability and transparency in decision-making workflows — linking simulation models, optimization datasets, and extracted knowledge to the final decisions made by diverse groups of decision-makers with varying preferences in both objective space and decision options.

3. Deeper insights enabled by integrating multi-objective optimization and simulation with the preference structures of multiple stakeholders.
4. Support for group decision-making and educational use cases through interactive exploration tools tailored to industrial users and students, respectively.

Our approach advances the VF-KDO concept by leveraging graph databases to manage interconnected optimization knowledge. Future work may further explore machine learning-based knowledge extraction, automated tuning of simulation-based optimization, and real-time optimization recommendations through graph-based reasoning.

Furthermore, it would be interesting to evaluate the system with a larger data set. Although the examples are enough to showcase the possibilities and advantages of our system, which would naturally amplify with larger amounts of data, some deeper insights might only be possible beyond a critical mass of data.

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