The World Avatar – a world model for facilitating interoperability

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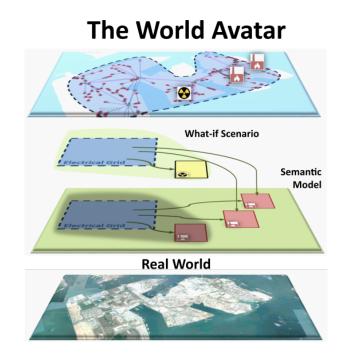
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Abstract

Digitalisation enhances communication and therefore offers new ways to achieve efficiency gains in science, technology and society at large. However, there are still many open questions around how digitalisation can contribute to a more sustainable environment and lifestyle. We believe that knowledge graph technology is a promising candidate with which this can be achieved. In this chapter, we present the World Avatar, a dynamic knowledge graph (dKG), and explain the main underlying concepts and principles. Using several use cases, two key fundamentally different aspects – control and design – are introduced and illustrated. In addition, we show how the World Avatar can improve interoperability between heterogeneous data formats as well as software, and thus enable cross-domain applications in wider contexts. Moreover, we highlight how the Parallel World framework can consider different scenarios and hence facilitate time-dependent what-if scenario analysis. All use cases show how interoperability between multiple domains involved in the complex decarbonisation process can contribute to CO_2 abatement of digitalisation.



Highlights

- Described the main underlying concepts and principles of the World Avatar project.
- Discussed how the World Avatar can improve interoperability.
- Highlighted how the Parallel World framework can facilitate what-if scenario analysis.
- Outlined the outlook for the World Avatar project.

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1 Introduction

Global warming has a drastic impact on the environment, health, the economy, biodiversity, infrastructure, food and water supplies *etc*. For instance, the World Health Organisation (WHO) reports that climate change is expected to cause approximately 250,000 additional deaths yearly between 2030 and 2050, and the direct damage to health is estimated to cost between USD 2 – 4 billion per annum by 2030 [28]. Carbon dioxide (CO₂) released due to fossil fuel combustion is reported as the overwhelming contributor to greenhouse gas (GHG) emissions. The National Oceanic and Atmospheric Administration (NOOA) reported that the global average atmospheric CO₂ in 2019 was 409.8 ppm – the highest in the past 800,000 years [2]. Moreover, the annual rate of increase in atmospheric CO₂ over the past 60 years is also noted to be approximately 100 times faster than previous natural increases. It has been estimated that if the global energy demand continues to grow and be satisfied predominately with fossil fuels, atmospheric CO₂ is projected to rise beyond 900 ppm by 2100 [2].

In 2017, the electricity and heat generation sector contributed 41.4% (13,603.3 million tonnes) to overall CO₂ emissions due to fuel combustion [1]. Therefore, the decarbonisation of energy provision plays a pivotal role in managing global GHG emissions and thus mitigating global warming. Inderwildi *et al.* [10] highlighted that the digitalisation of energy systems using cyber-physical systems (CPS) can alter the marginal abatement cost curve (MACC) towards higher CO₂ abatement potentials. This implies that CPS have the potential to increase the efficiency of energy provision and industrial production, and hence possess great emissions reduction potential. This potential increases further when CPS are combined with Artificial Intelligence (AI).

To fully unleash this potential, addressing and overcoming the current challenge of low interoperability between multiple domains involved in the complex decarbonisation process is a prerequisite. The challenge is attributed to the presence of information silos, *e.g.* disconnected data lakes and AIs arising from heterogeneity of data and services (software and tools), and the non-uniqueness of data *i.e.* data duplication and inconsistency. Any complex process involves collating large amounts of information, tools and models from multiple domains, which may comprise varying degrees of model resolution that are subjected to complex interaction loops. These information, tools and models typically have features of syntax and semantic heterogeneity, making communication across domains' boundaries challenging. Consequently, a substantial amount of effort is commonly required to process and convert the different data formats, and to navigate through a dynamic information base for decision making. This results in the process being slow and labour-intensive, and does not make the best use of the available data, which in turn narrows its potential.

Doan *et al.* [5] described how semantic data heterogeneity can be a major bottleneck for data integration. The semantic web and its technologies, such as Resource Description Framework (RDF) and Web Ontology Language (OWL), offer the potential to increase the interoperability by formalising the representation of data and services. Semantic web technologies are standardised, provide a uniform way to query and link data, and have been approved for many years. In addition to being a suitable candidate for data integration, semantic web technologies provide unique features of knowledge management

and reasoning in comparison to other approaches. This approach enables data and services that are often siloed at present to understand and communicate with each other, and thus use each other's functionalities. In particular, the ontology-based knowledge graphs demonstrate good prospects with the emergence of the first practical implementations in the context of the "World Avatar" project [6, 7, 10, 33, 34].

The purpose of this chapter is to:

- Introduce the concepts of the World Avatar project which is based on dynamic ontology-based knowledge graphs;
- Describe use cases that demonstrate the application of these concepts, emphasising two fundamentally different aspects control and design.

2 The World Avatar – A Dynamic Knowledge Graph

A knowledge graph represents information by making use of the principles of Linked Data as employed in the semantic web, where concepts correspond to vertices and relationships between concepts correspond to edges of the graph. As a representation of information, the key distinguishing feature of a knowledge graph is that individual aspects of the information are linked to each other. In the World Avatar project, this representation is implemented by means of ontologies, which formalise the definition of concepts and their relationships through collections of subject-predicate-object triples. The World Avatar concept intends to capture the idea of representing every aspect of the real world in a digital "mirror" world. This is essentially an extension of the Digital Twin notion, where, taking an example from Industry 4.0, a device or a unit operation in an industrial process has a corresponding virtual representation. A natural logical continuation is the application of this approach beyond the industrial context – the virtualisation of any abstract concept or process, similar to the extension of the Internet of Things to the Internet of Services and beyond.

The "J-Park Simulator" (JPS)¹ [6] is an implementation and subset of the World Avatar concept. Figure 1 illustrates its main underlying principles. The World Avatar started with a focus on virtualising industrial operations within the Jurong Island Eco-Industrial Park (EIP) in Singapore [11, 19, 20, 31] using the concepts mentioned in [12], but has since expanded well beyond this original scope. Fundamental to the World Avatar is a dynamic knowledge graph (dKG) that is envisioned as general-purpose and all-encompassing. In the World Avatar, the Linked Data concept is implemented using Internationalised Resource Identifiers (IRIs)², a protocol element that complements Uniform Resource Identifiers (URIs). Essentially, IRIs are generalised web addresses that are used to point to a resource on the Web [29]. Various modular domain ontologies have been employed in the World Avatar. These include OntoCAPE (for computer-aided process engineering [17]), OntoEIP (for EIPs [30–32]), OntoPowSys (for power systems [4]) and OntoCityGML (for 3D models of cities and landscapes [6]). In the chemistry domain, ontologies

http://www.theworldavatar.com/

²https://www.w3.org/International/O-URL-and-ident.html

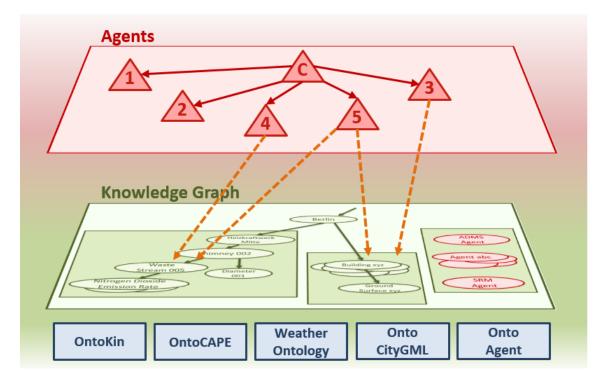


Figure 1: An illustration of the main principles for the dynamic knowledge graph: a) modular domain ontologies (blue), b) instances of various types of agents (atomic, composition and composite) (red node), and c) active agents (red triangles) operating on the knowledge graph and interacting with each other. "Agent" refers to software, methods, applications and services etc. that utilise semantic web technologies and operate on the knowledge graph to read/write, estimate, simulate, optimise and/or query etc. to fulfil specific objectives. Reproduced from [6].

were developed to semantically describe the subdomains of quantum chemistry calculations (OntoCompChem [13]), species (OntoSpecies [9]), and chemical kinetic reaction mechanisms (OntoKin [8]). Furthermore, the use of Linked Data allows the World Avatar knowledge graph to connect to various subgraphs of the Linked Open Data (LOD) Cloud³, in particular DBpedia⁴ [14], and leverage the wealth of data available on the Internet.

Beyond mere data representation, the World Avatar contains an ecosystem of software agents that act autonomously and continuously on the knowledge graph, constantly updating it and thus making it evolve in time. Crucially, the agents themselves are part of the knowledge graph, governed by an agent ontology (OntoAgent [33]). In particular, agents were developed for automatic agent discovery and composition [33], *i.e.* agents that create new, composite agents for more complex tasks. Furthermore, in order to facilitate the use of agents and simplify the identification of an agent suitable for a specific task in an agent-rich environment (where an abundance of services is available), an agent marketplace based on blockchain technology and Smart Contracts was established [34].

³https://lod-cloud.net/

⁴https://wiki.dbpedia.org/

With its generic, all-purpose design based on ontologies and autonomous agents, the World Avatar improves interoperability between heterogeneous data formats as well as software, and thus enables cross-domain applications in wider contexts. For example, the World Avatar has been employed in the optimal site selection for modular nuclear power plants [3] and simulation of atmospheric dispersion of pollutants in emissions use cases involving power plants [6]. In addition, the World Avatar provides the capability to consider different scenarios for scenario planning via the usage of the "Parallel World" framework [7].

3 Use Cases

In this section, several use cases that demonstrate the application of a dKG will be presented. These use cases are associated with Singapore and primarily with its Jurong Island EIP due to the above-mentioned reason. However, in principle, the application of the dKG is not restricted to these contexts – the dKG could be extended to, for instance, other countries and sectors.

The five use cases have been categorised into two groups to introduce and illustrate two fundamentally different aspects of the World Avatar concept – control and design. The first three use cases demonstrate how digital twinning in the context of a dKG can reduce costs and energy via intelligent control strategies. The subsequent two use cases exemplify how the Parallel World framework can be employed to create a "live" digital world *i.e.* a scenario that enables the investigation of different technology alternatives and the effect of policies on technology transition.

3.1 Digital Twinning – Intelligent Control Strategies

Singapore, an island city-state in Southeast Asia, is a modern city with highly developed infrastructure. Apart from being one of the world's most densely populated countries [26], with a population of 5.69 million people [23], Singapore also hosts one of the world's busiest ports and leading energy and chemicals hubs. Situated off the southern coast of Singapore, Jurong Island is the core of Singapore's energy and chemicals industry. With a land area of 31 square kilometres, Jurong Island is home to over 100 global petroleum, petrochemical and speciality chemical companies [24] and has attracted over \$\$50 billion worth of investments [25]. Some of these companies such as Evonik, BASF, ExxonMobil, Linde, Shell *etc.* are prominent players in the field. In 2014, with 1.5 million barrels of oil being refined per day on Jurong Island, Singapore is one of the top ten exporters of refined oil products in Asia [25]. In 2015, the energy and chemicals industry also contributed \$\$81 billion – about a third of Singapore's total manufacturing output [25]. These figures illustrate the importance of the energy and chemicals industry to Singapore's economy. Unfortunately, the energy and chemicals industry is also the largest source of emissions in Singapore.

As mentioned in Section 2, the World Avatar project started with a focus on virtualising industrial operations within Jurong Island. In the following subsections, three use cases

which comprise multiple domains such as energy, electrical and chemical networks, with varying scales and degrees of detail, will demonstrate how digital twinning and intelligent control strategies in the context of a dKG can increase the efficiency of energy provision and CO_2 abatement potentials.

3.1.1 Control Strategy – Depropaniser section

Although chemical processes and electrical power system operations are usually analysed separately, in reality, any change in the chemical processes will be reflected in the corresponding electrical load demand profile and might affect the transient stability and power quality of the electrical system. In this use case, the dKG is utilised to recommend the control strategy for the feed flow rate of the depropaniser section within a typical natural gas processing plant. The relevant chemical and electrical aspects have been modelled using the software gPROMS⁵ and MATLAB⁶ respectively. The two programs have been packaged as two distinct agents that can apply the semantic web stack to read and understand information from the dKG and modify its data values. The real power consumed by the chemical processes is used to couple the chemical and electrical systems. The dKG establishes machine-to-machine (M2M) communications between the two typically siloed systems via an agent framework, and ontology called "OntoTwin". The OntoTwin ontology is developed based on combining and extending the aforementioned OntoPowsys and OntoEIP ontologies. The agent framework employs Description Logics (DL), SPARQL Inferencing Notation⁷ (SPIN) reasoning techniques, as well as detailed models of the selected chemical and electrical systems (as shown in Figure 2) to investigate the interactions between the two systems. As operating constraints such as product and power qualities have been incorporated into the framework, the framework is capable of predicting any constraint violation arising from the proposed control strategy - even before their implementations.

Moreover, a comparative study was conducted with two different ratings of transformer -300 kVA and 500 kVA (standard design). The study revealed that by adopting the recommended control strategy, a lower-rated and thus cheaper transformer *i.e.* 300 kVA will be sufficient for the specified purpose. This was estimated to translate to a cost saving of approximately EUR 40,000. The use case illustrates how digital twinning (of the depropaniser section) in the context of a dKG can provide smooth operation and better design through: 1) maintaining both the product and power qualities within their desired operating ranges, thus reducing the quantity of off-spec products and downtime; and 2) the potential to utilise a lower-rated transformer attributed to the adoption of the recommended control strategy.

3.1.2 Control Strategy – Heat and Power Dispatch

Combined Heat and Power (CHP) cogeneration system is an energy-efficient technology that concurrently produces electrical and useful thermal energy such as steam or hot wa-

⁵https://www.psenterprise.com/products/gproms

⁶https://www.mathworks.com/products/matlab.html

⁷https://spinrdf.org/

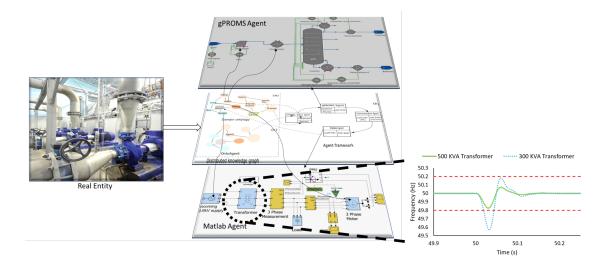


Figure 2: Digital twin of the depropaniser section within a typical natural gas processing plant.

ter. In conventional electricity generation, approximately two-thirds of the energy used is dissipated in the form of heat to the atmosphere [27]. Through capturing and transforming this waste heat, CHP can attain energy efficiency of over 80% [27]. Consequently, CHP is commonly deployed at sites that require both electrical and thermal energy *e.g.* Jurong Island. In this use case, the dKG is utilised to determine the optimal scheduling for the operation of the Combined Cycle Gas Turbines (CCGTs) within a grid. The objective is to propose heat and power dispatch to fulfil both the thermal and electrical loads, as well as grid constraints, while minimising the overall CO_2 emissions. A detailed digital twin of an electrical network has been developed and described with the OntoPowSys ontology [4] for this purpose. Figure 3 visualises a subset of this digital twin – representation of the transmission grid. Comparing with uncontrollable cogeneration units *i.e.* priority is given to electrical energy, it is concluded that significant CO_2 emissions reduction can be attained via the efficient power dispatch strategy, in particular for higher heat load levels. More details on the implementation and results can be found in references [21] and [22].

3.1.3 Control Strategy – Energy Demand Side Management

Distributed energy resources (DERs) are technologies that primarily consist of small, modular energy generation and storage systems. DERs may either be connected to the local electric power grid or as stand-alone applications [18]. With the growing attention on renewable energy, generation technologies such as wind turbines and photovoltaics are also being incorporated into the DERs. In the meantime, technology advancements on the energy demand side will result in the automation of smart controllable loads and the growth in demand side management schemes such as demand response [16].

Building upon the work in [16], an energy demand side management framework was developed in the context of a dKG. The objective of this agent framework is to reduce the peak to average ratio, which in turn leads to lower stress on the main grid and hence provides cost savings for the consumers. The current agent framework considers the

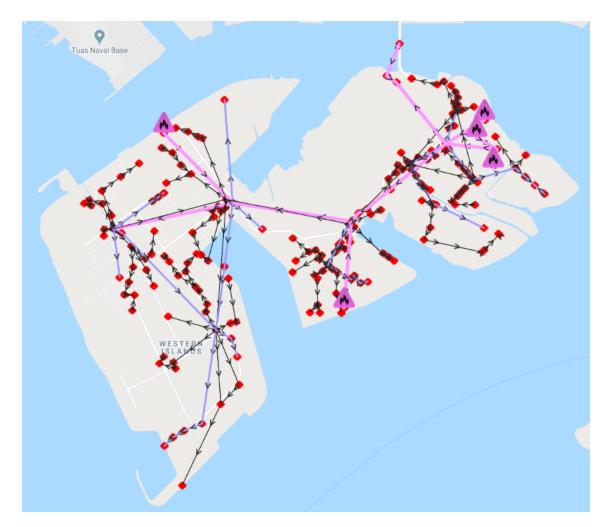


Figure 3: Digital Twin – Transmission Grid. The coloured lines represent the transmission lines in the electrical network that connect buses which are represented by the red points. Different coloured transmission lines represent different voltage levels: pink represents 230 kV, purple represents 66 kV and black represents 22 kV. The arrow indicates the direction of the current flow from one bus to another within the network. The gas symbols denote the power plants.

forecasted renewable energy generated by solar photovoltaic cells, three types of energy consumers (residential, commercial and industrial) as well as their demand flexibilities. The dKG establishes communications between the various players and data via the OntoPowSys ontology and an agent framework that employs a game theory modelling approach. Furthermore, energy trading based on the optimised energy profiles is secured via the use of blockchain technology. This use case illustrates how digital twinning (of the players) in the context of a dKG can: 1) reduce the overall CO_2 emissions by increasing penetration of renewable energy sources while fulfilling the players' demand constraints; and 2) through the application of blockchain technology, create a seamless, secured and efficient energy system that lowers the threshold of participation in the electricity market for small players.

3.2 Digital Twinning – Intelligent Design Strategies

In a complex decision environment, decision-making processes face the challenge of predicting and/or estimating the impact of any decision. Scenario analysis facilitates decision making by exploring and presenting different options and their corresponding outcomes and implications. As mentioned in Section 2, the dKG provides the capability to consider different scenarios via the usage of the Parallel World framework. The underlying knowledge graph based design of the World Avatar project and semantic web technologies allow instances (from different sources) within the dKG to be annotated with additional information (e.g. versioning and provenance data). This corresponds to the "live" Parallel World concept which keeps entities involved in the same scenario together and delegates their access, queries and updates on the dKG to a scenario-specific portion of the dKG. The scenario-specific portion only overshadows the portion of the dKG where modifications are necessary. Entities that are unchanged remain connected to the "Base World" of the dKG. This architecture allows entities involved in the same scenario to: 1) maintain connections to the Base World *i.e.* modifications in the Base World will be reflected in the Parallel Worlds; and 2) operate in a "secured portion" of the dKG without interfering with other entities or impacting the Base World.

The Parallel World framework also enables data to be linked and queried in a highly flexible manner. Consequently, the Parallel World concept is able to assist in design space exploration and its management by allowing the modification of relevant data and parameters, and storing the different versions and scenario results in the dKG without mutual interference (*i.e.* where each world is configured with its own data and describes a potential state). More details on the Parallel World framework and its implementation can be found in reference [7].

3.2.1 Design Strategy – Energy Storage Technology Selection and Placement

One of the major challenges for increasing the penetration of renewable energy sources is their availability and intermittency, which can be addressed with the deployment of energy storage systems (ESS). ESS involve converting excess energy to a form that can be stored *e.g.* electrochemical (lithium-ion battery) or mechanical (pumped hydro), and transforming the stored energy back into electricity when it is required. Driven by the growing attention on ESS, many types of ESS and applications have emerged during the last few decades. Consequently, a systematic framework that facilitates the selection of suitable energy storage technologies among the increasing options is necessary [15].

Building upon the work in [15], an energy storage technology selection and placement framework was developed in the context of a dKG. The objective of the framework is to recommend appropriate energy storage technology based on a variety of factors such as technological feasibility, maturity, installation cost, *etc.* Once the energy storage technology is determined, the optimal placement of the ESS for a given grid topology to minimise distribution system losses is established based on the system loss sensitivity index with respect to the ESS parameters. The current agent framework considers six types of energy storage technologies and has been applied to the aforementioned digital twin of an electrical network (Section 3.1.2). The OntoPowSys ontology was extended to describe and

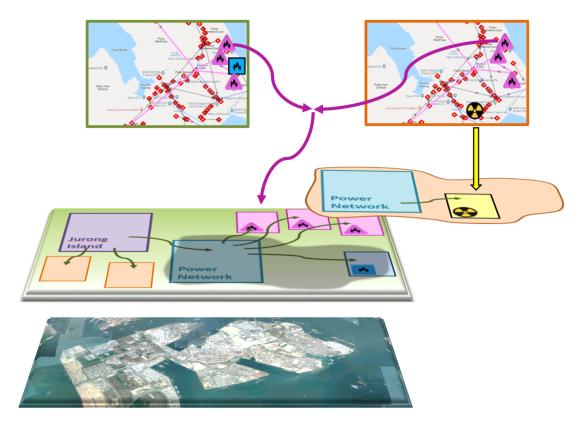


Figure 4: Parallel World concept for what-if scenario analysis. Entities are represented and linked semantically in the knowledge graph. Reproduced from [7].

instantiate the relevant energy storage technologies in the dKG. This use case illustrates how digital twinning (of the electrical network and different energy storage technologies) in the context of a dKG can: 1) recommend optimal ESS selection and placement strategy; and 2) reduce the overall CO_2 emissions by encouraging penetration of renewable energy sources.

3.2.2 Design Strategy – Effect of Carbon Tax on Technology Transition

A carbon tax is a tax levied on the combustion of fossil fuels *e.g.* coal, oil and natural gas, and is associated with the global warming potentials of its emissions. The carbon tax aims to motivate the transition to alternative clean energy by discouraging the use of fossil fuels whose combustion generates GHG (primarily CO_2). In this use case, the dKG is utilised to address the following questions: 1) For a set of conditions *e.g.* a generator's characteristics (design capacity, carbon emission factor, capital cost, fuel cost *etc.*), a project's life span, depreciation rate and load profiles, what is the minimum value of carbon tax required to motivate (*i.e.* it becomes profitable) the replacement of existing power plant(s) with small modular nuclear reactors (SMRs); 2) which existing power plant(s) / generator(s) need to be replaced; 3) what are the required number and optimal locations for the new SMRs; and 4) how to connect these SMRs to the existing transmission grid. The current agent framework has been applied to the aforementioned digital twin of an electrical

network (Section 3.1.2) which comprises six oil and 22 natural gas generators. Similarly, the OntoPowSys ontology was extended to describe and instantiate the relevant SMRs and generators in the dKG. When the carbon tax is increased from \$5 to \$170, the oil generators are replaced with SMRs in the Parallel World. The corresponding estimated CO_2 emissions and types of generators are updated automatically in the dKG to reflect these changes. Subsequently, an Optimal Power Flow (OPF) agent is invoked to minimise the overall operating cost. More details on the implementation and results can be found in references [3] and [7]. This use case illustrates how digital twinning in the context of a dKG can allow decision-makers to better understand the effect of policy instruments such as carbon tax and therefore helps to move faster towards a low-carbon economy.

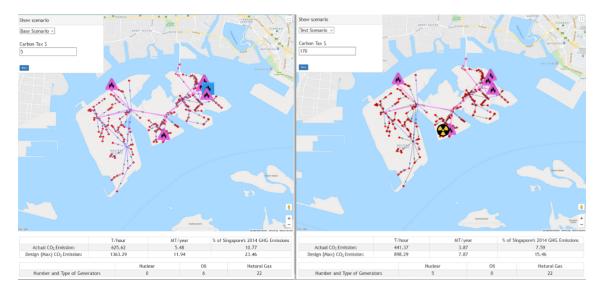


Figure 5: The illustration on the left depicts the original electrical network and the illustration on the right depicts the modified electrical network. Blue square denotes oil generator, pink triangles denote natural gas generators, and radiation symbol denotes small modular nuclear reactor.

4 Outlook and Conclusion

The main underlying concepts and principles of the World Avatar project – which is based on dKG – have been described in this chapter. Using several use cases, two key fundamentally different aspects, control and design, have also been introduced and illustrated. In addition, it was discussed how the World Avatar can improve interoperability between heterogeneous data formats as well as software, and thus enables cross-domain applications in wider contexts. Moreover, it was highlighted how the Parallel World framework can consider different scenarios and hence facilitate what-if scenario analysis.

Despite the above-mentioned work, there are many open questions to be answered and more work to be done in order to advance and further leverage the potential of the World Avatar concepts. Some of these areas are described as follows:

- 1. Extend the dKG with additional domains and their corresponding ontologies *e.g.* financial, health and safety, and new instances *e.g.* digital twin of the European and United Kingdom electrical network.
- 2. Create and integrate more software agents for various application domains into the dKG. This includes the use of machine learning algorithms to increase computational speed and intelligence.
- 3. Increase the dKG's connectivity and application to real/physical systems *e.g.* via sensors and actuators. This includes utilising satellite data and other publicly available data sources.
- 4. Resolve conflicting and incomplete domain ontologies *e.g.* through ontology matching techniques employing natural language processing and machine learning.
- 5. Improve the current dKG's query, access and writing speed e.g. via the use of indexing.
- 6. Enhance the capability, performance and scalability of the semantic agent composition framework to facilitate automatic agent discovery and composition.
- 7. Include cybersecurity and resilience aspects in the dKG.
- 8. Introducing goals that guarantee human-friendly operation and design, including an ontology for the UN Sustainable Development Goals, has been identified as the first step in this direction.

Despite this long list of necessary improvements, we conclude that the World Avatar project has the potential to address and overcome the challenge of low interoperability between multiple domains involved in the complex decarbonisation process, therefore realising the CO_2 abatement potential of digitalisation.

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References

- [1] International Energy Agency. CO₂ Emissions from Fuel Combustion Highlights, 2019. URL https://iea.blob.core.windows.net/assets/ eb3b2e8d-28e0-47fd-a8ba-160f7ed42bc3/CO2_Emissions_from_Fuel_ Combustion_2019_Highlights.pdf. Accessed 22 October 2020.
- [2] National Oceanic and Atmospheric Administration. Climate Change: Atmospheric Carbon Dioxide, 2020. URL https://www.climate.gov/newsfeatures/understanding-climate/climate-change-atmosphericcarbon-dioxide. Accessed 22 October 2020.
- [3] A. Devanand, I. A. Karimi, and M. Kraft. Optimal site selection for modular nuclear power plants. *Computers & Chemical Engineering*, 125:339–350, 2019. doi:10.1016/j.compchemeng.2019.03.024.
- [4] A. Devanand, G. Karmakar, N. Krdzavac, R. Rigo-Mariani, Y. S. Foo, I. A. Karimi, and M. Kraft. OntoPowSys: A power system ontology for cross domain interactions in an eco industrial park. *Energy and AI*, 1:100008, 2020. doi:10.1016/j.egyai.2020.100008.
- [5] A. Doan, A. Halevy, and Z. Ives. *Principles of Data Integration*. Morgan Kaufmann, 2012.
- [6] A. Eibeck, M. Q. Lim, and M. Kraft. J-Park Simulator: An ontology-based platform for cross-domain scenarios in process industry. *Computers & Chemical Engineering*, 131:106586, 2019. doi:10.1016/j.compchemeng.2019.106586.
- [7] A. Eibeck, A. Chadzynski, M. Q. Lim, K. Aditya, L. Ong, A. Devanand, G. Karmakar, S. Mosbach, R. Lau, I. A. Karimi, and et al. A parallel world framework for scenario analysis in knowledge graphs. *Data-Centric Engineering*, 1:e6, 2020. doi:10.1017/dce.2020.6.
- [8] F. Farazi, J. Akroyd, S. Mosbach, P. Buerger, D. Nurkowski, M. Salamanca, and M. Kraft. OntoKin: An ontology for chemical kinetic reaction mechanisms. *Journal of Chemical Information and Modeling*, 60(1):108–120, 2020. doi:10.1021/acs.jcim.9b00960.
- [9] F. Farazi, N. Krdzavac, J. Akroyd, S. Mosbach, A. Menon, D. Nurkowski, and M. Kraft. Linking reaction mechanisms and quantum chemistry: An ontological approach. *Computers & Chemical Engineering*, 137:106813, 2020. doi:10.1016/j.compchemeng.2020.106813.
- [10] O. Inderwildi, C. Zhang, X. Wang, and M. Kraft. The impact of intelligent cyberphysical systems on the decarbonization of energy. *Energy & Environmental Science*, 13(3):744–771, 2020. doi:10.1039/C9EE01919G.
- [11] M. J. Kleinelanghorst, L. Zhou, J. Sikorski, Y. S. Foo, L. K. Aditya, S. Mosbach, I. A. Karimi, R. Lau, and M. Kraft. J-Park Simulator: Roadmap to smart eco-industrial parks. *Proceedings of the Second International Conference*

on Internet of Things, Data and Cloud Computing (ICC '17), pages 1–10, 2017. doi:10.1145/3018896.3025155.

- [12] M. Kraft and S. Mosbach. The future of computational modelling in reaction engineering. *Philosophical Transactions*, 368:3633–3644, 2010. doi:10.1098/rsta.2010.0124.
- [13] N. Krdzavac, S. Mosbach, D. Nurkowski, P. Buerger, J. Akroyd, J. Martin, A. Menon, and M. Kraft. An ontology and semantic web service for quantum chemistry calculations. *Journal of Chemical Information and Modeling*, 59(7):3154– 3165, 2019. doi:10.1021/acs.jcim.9b00227.
- [14] J. Lehmann, R. Isele, M. Jakob, A. Jentzsch, D. Kontokostas, P. N. Mendes, S. Hellmann, M. Morsey, P. van Kleef, S. Auer, and C. Bizer. DBpedia – A large-scale, multilingual knowledge base extracted from Wikipedia. *Semantic Web*, 6(2):167– 195, 2015. doi:10.3233/SW-140134.
- [15] L. Li, P. Liu, Z. Li, and X. Wang. A multi-objective optimization approach for selection of energy storage systems. *Computers & Chemical Engineering*, 115:213 – 225, 2018. doi:10.1016/j.compchemeng.2018.04.014.
- [16] Y. Li, W. Yang, P. He, C. Chen, and X. Wang. Design and management of a distributed hybrid energy system through smart contract and blockchain. *Applied Energy*, 248:390 – 405, 2019. doi:10.1016/j.apenergy.2019.04.132.
- [17] W. Marquardt, J. Morbach, A. Wiesner, and A. Yang. OntoCAPE A Re-Usable Ontology for Chemical Process Engineering. Springer-Verlag Berlin Heidelberg, 1st edition, 2010. doi:10.1007/978-3-642-04655-1.
- [18] National Renewable Energy Laboratory. Using Distributed Energy Resources, 2002. URL https://www.nrel.gov/docs/fy02osti/31570.pdf. Accessed 22 October 2020.
- [19] M. Pan, J. Sikorski, C. A. Kastner, J. Akroyd, S. Mosbach, R. Lau, and M. Kraft. Applying Industry 4.0 to the Jurong Island eco-industrial park. *Energy Procedia*, 75:1536–1541, 2015. doi:10.1016/j.egypro.2015.07.313.
- [20] M. Pan, J. Sikorski, J. Akroyd, S. Mosbach, R. Lau, and M. Kraft. Design technologies for eco-industrial parks: From unit operations to processes, plants and industrial networks. *Applied Energy*, 175:305–323, 2016. doi:10.1016/j.apenergy.2016.05.019.
- [21] R. Rigo-Mariani, K. V. Ling, and J. Maciejowski. A clusterized energy management with linearized losses in the presence of multiple types of distributed generation. *International Journal of Electrical Power & Energy Systems*, 113:9 – 22, 2019. doi:10.1016/j.ijepes.2019.04.049.
- [22] R. Rigo-Mariani, C. Zhang, A. Romagnoli, M. Kraft, K. V. Ling, and J. Maciejowski. A combined cycle gas turbine model for heat and power dispatch subject to grid constraints. *IEEE Transactions on Sustainable Energy*, 11(1):448–456, 2020. doi:10.1109/TSTE.2019.2894793.

- [23] Singapore Department of Statistics. Singstat, 2020. URL https://www.singstat.gov.sg/. Accessed 22 October 2020.
- [24] Singapore Economic Development Board (EDB). Singapore: A leading manufacturing hub, 2018. URL https://www.edb.gov.sg/en/news-andevents/insights/innovation/singapore-a-leading-manufacturinghub.html. Accessed 22 October 2020.
- [25] Singapore Economic Development Board (EDB). The Right Chemistry, 2020. URL https://www.edb.gov.sg/en/our-industries/energy-andchemicals.html. Accessed 22 October 2020.
- [26] The World Bank Group. Population Density (people per sq. km of land area), 2018. URL https://data.worldbank.org/indicator/EN.POP.DNST. Accessed 22 October 2020.
- [27] United States Environmental Protection Agency. Combined Heat and Power (CHP) Partnership, 2019. URL https://www.epa.gov/chp/what-chp. Accessed 22 October 2020.
- [28] World Health Organisation. Climate change and health, 2018. URL https://www.who.int/news-room/fact-sheets/detail/climate-change-and-health. Accessed 22 October 2020.
- [29] World Wide Web Consortium. An Introduction to Multilingual Web Addresses, 2008. URL https://www.w3.org/International/articles/idn-andiri/. Accessed 22 October 2020.
- [30] C. Zhang, A. Romagnoli, L. Zhou, and M. Kraft. Knowledge management of ecoindustrial park for efficient energy utilization through ontology-based approach. *Applied Energy*, 204:1412–1421, 2017. doi:10.1016/j.apenergy.2017.03.130.
- [31] L. Zhou, M. Pan, J. J. Sikorski, S. Garud, L. K. Aditya, M. J. Kleinelanghorst, I. A. Karimi, and M. Kraft. Towards an ontological infrastructure for chemical process simulation and optimization in the context of eco-industrial parks. *Applied Energy*, 204:1284–1298, 2017. doi:10.1016/j.apenergy.2017.05.002.
- [32] L. Zhou, C. Zhang, I. A. Karimi, and M. Kraft. An ontology framework towards decentralized information management for eco-industrial parks. *Computers & Chemical Engineering*, 118:49–63, 2018. doi:10.1016/j.compchemeng.2018.07.010.
- [33] X. Zhou, A. Eibeck, M. Q. Lim, N. Krdzavac, and M. Kraft. An agent composition framework for the J-Park Simulator – a knowledge graph for the process industry. *Computers & Chemical Engineering*, 130:106577, 2019. doi:10.1016/j.compchemeng.2019.106577.
- [34] X. Zhou, M. Q. Lim, and M. Kraft. A smart contract-based agent marketplace for the J-Park Simulator – a knowledge graph for the process industry. *Computers & Chemical Engineering*, 139:106896, 2020. doi:10.1016/j.compchemeng.2020.106896.