

Digital Twin - exploring the basics

The concept of digital twins is not new, but rather built on ideas that have been explored for the last couple of decades. The technology (compute power, data management & analytics, etc..) and thinking (increasing regulatory and community acceptance of digital approaches to science) have finally hit an inflection point that makes in silico modeling attainable in a cost effective manner.

What this now unlocks is a new opportunity set in the form of machine accessible data, as well as integration of the data sets / ontologies across the target systems / interactions. The need to get to a standardized mechanism to make these data available is tied to the FAIR Data work, and an important dimension to Digital Twin.

Digital twins vs. simulations

Although simulations and digital twins both utilize digital models to replicate a system's various processes, a digital twin is actually a virtual environment, which makes it considerably richer for study. The difference between digital twin and simulation is largely a matter of scale: While a simulation typically studies one particular process, a digital twin can itself run any number of useful simulations in order to study multiple processes.

SOURCE: [IBM](#) , [WHAT IS A DIGITAL TWIN](#)

At it's heart, the idea of a digital twin is to reproduce a system in a "runnable" computer model. This oversimplifies the idea, but is a useful construct to think about the problem space and the opportunity it presents. If you can take a scientific instrument, and fully model it in silico, you can then run data sets through it virtually - this makes the assumption that both the inbound and outbound data are available in a machine usable format - something that is tied to this work.

Digital twin is an interdisciplinary research field which includes engineering, computer science, automation and control, and so on. But due to the multidisciplinary nature of the field, it also touches on materials science, communication, operations management, robotics, medicine and other disciplines. A keyword analysis indicates that digital twin, 'smart manufacturing', 'big data', 'cyber-physical system', and 'digital economy' are closely related fields.

SOURCE: "INNOVATIONS IN DIGITAL TWIN RESERACH" FROM [NATURE PORTFOLIO](#)

The article in nature.com is an interesting piece in that it ties together the many dimensions in this field of research. We can't think of "Digital Twin" as a single entity opportunity, rather to fully realize the potential, we need to look at it as a part of an emerging "virtual capability ecosystem" with applications back to the real

world. The value is realized in lower long term costs with increased innovation driven by reduced cost and cycle times, accompanied by increases in application of AI / ML on these models to gain targeted insights that more sharply focus the bench work.

Track the past and help predict the future of any connected environment

SOURCE: AZURE DIGITAL TWINS

The ability to create learning models for these Digital Twins will improve the accuracy and usefulness of the models over time, and that feedback loop will be a critical part of design. While the industry is maturing, we are seeing more vendors coming to the table with solutions in this space. One of the interesting things to watch is how we as an industry continue to drive open standards in support of these ideas to avoid the traps of “vendor lock in” that were so prevalent in the past.

Ontologies as applied to FAIR data

(The I in FAIR)

Ontologies provide a common structure to bring disparate data together – for this post I will refer to the definition of Ontology from Tom Gruber below – emphasis added by me. Note the last highlighted statement as a critical bit with significant implications in the implementation of systems in support of scientific processes. Having led and survived many data and systems integration efforts over the years, one of the most challenging aspects is hidden in this last statement. Changing data format, naming, etc... at the source is often met with almost religious fervor as change had wide-ranging implications to linked analysis, and multiple stakeholders have disparate needs or views of the data in question. The idea of an abstraction layer to bring these data together is nothing new, and this approach is a natural evolution in my mind. We are recognizing as an industry that isolated data is useful in context, but far more powerful when shared. To attain that goal, we need a common vocabulary and structure – enter the domain ontologies we can map to.

In the context of computer and information sciences, an **ontology defines a set of representational primitives with which to model a domain of knowledge or discourse**. The representational primitives are typically classes (or sets), attributes (or properties), and relationships (or relations among class members). The definitions of the representational primitives include information about their meaning and constraints on their logically consistent application. In the context of database systems, **ontology can be viewed as a level of abstraction of data models, analogous to hierarchical and relational models, but intended for modeling knowledge about individuals, their**

attributes, and their relationships to other individuals. Ontologies are typically specified in languages that allow abstraction away from data structures and implementation strategies; in practice, the languages of ontologies are closer in expressive power to first-order logic than languages used to model databases. For this reason, ontologies are said to be at the “semantic” level, whereas database schema are models of data at the “logical” or “physical” level. **Due to their independence from lower level data models, ontologies are used for integrating heterogeneous databases, enabling interoperability among disparate systems,** and specifying interfaces to independent, knowledge-based services.

[HTTPS://TOMGRUBER.ORG/WRITING/DEFINITION-OF-ONTOLOGY.PDF](https://tomgruber.org/writing/definition-of-ontology.pdf)

The ontology provides a navigable structure to the data relationships that will be consistent across all sources in scope of reference. This is the critical bit to derive value from the data - moving it from isolated to interoperable, and supporting the rest of the FAIR principles. Access control is often a critical bit when joining / sharing data, especially anything that can be used to form a conclusion that may be subject to challenge or reinterpretation absent context. Ontology based access can be used to support these access controls given the proper structure. While outside the scope of this surface level post, you can [read more from MIT Press Direct here](#) on that topic.

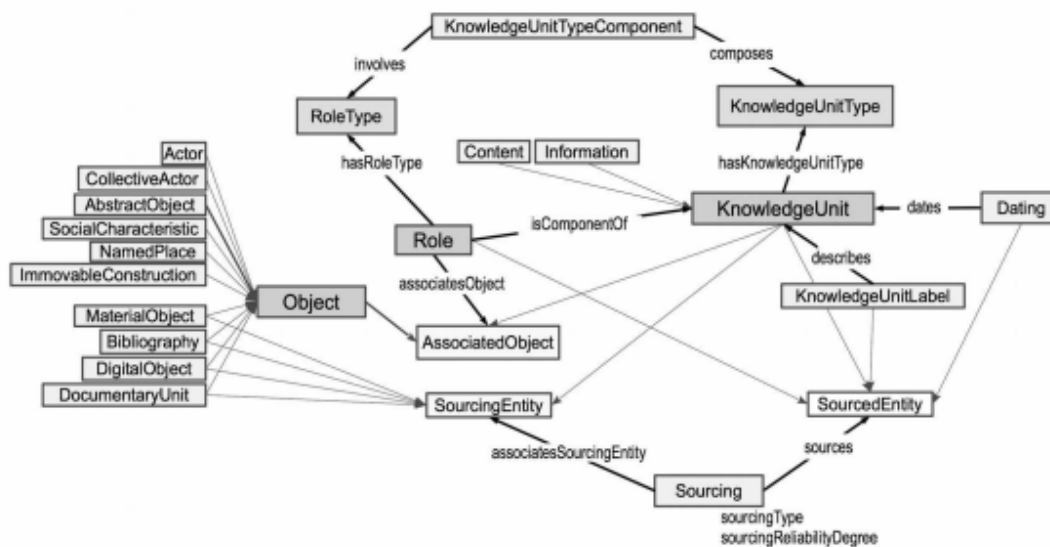


Fig. 1. Ontology of the symogih.org project -version 0.2.1

<http://www.semantic-web-journal.net/system/files/swj2523.pdf>

Mapping these ontologies and related data sets to a graph database and unlocking the power of the relationship hierarchy inferred through the ontology mapping, secured through the same, provides a rich foundation to build a query and interaction layer. There are challenges to be solved throughout this process, and this posts scratches the surface and provides some context / links, but it does help frame jumping off point for these ideas along with connections to papers and resources with the “rest of the story” as [Paul Harvey](#) would say.

References:

1. Tom Gruber (2008), Ontology. Entry in the *Encyclopedia of Database Systems*, Ling Liu and M. Tamer Özsu (Eds.), Springer-Verlag, 2009. <https://tomgruber.org/writing/definition-of-ontology>
2. Giancarlo Guizzardi; Ontology, Ontologies and the “I” of FAIR. *Data Intelligence* 2020; 2 (1-2): 181-191. doi: https://doi.org/10.1162/dint_a_00040
3. Poveda-Villalón, María & Espinoza-Arias, Paola & Garijo, Daniel & Corcho, Oscar. (2020). Coming to Terms with FAIR Ontologies. https://www.researchgate.net/publication/344042645_Coming_to_Terms_with_FAIR_Ontologies
A. [Direct link in case above link fails](#)
4. Francesco Beretta, 06/30/2020. A challenge for historical research: making data FAIR using a collaborative ontology management environment (OntoME) <http://www.semantic-web-journal.net/content/challenge-historical-research-making-data-fair-using-collaborative-ontology-management-0>
A. [Direct link to paper in case above link fails](#)
5. Christopher Brewster, Barry Nouwt, Stephan Raaijmakers, Jack Verhoosel; Ontology-based Access Control for FAIR Data. *Data Intelligence* 2020; 2 (1-2): 66-77. doi: https://doi.org/10.1162/dint_a_00029
6. Tim Berners-Lee, Date: 2006-07-27, last change: \$Date: 2009/06/18 18:24:33 \$, Status: personal view only. Editing status: imperfect but published. <https://www.w3.org/DesignIssues/LinkedData.html>

Is your Scientific Data FAIR

For many years, we have seen the proliferation of data as we increasingly instrument our scientific processes. We have developed a diverse landscape of tools and processes, making significant leaps from paper based documentation, but created a new nightmare of integration and complex analysis. The FAIR initiative or set of principles is a framework to reduce that complexity through the application of a core set of principles outlined below, making data machine readable across sources. This unlocks the data from the proprietary structure and system walls, and offers a foundation to build interconnected analysis and insights.

Reference this excerpt from the abstract here that summarizes quite nicely what the objective is:

There is an urgent need to improve the infrastructure supporting the reuse of scholarly data. A diverse set of stakeholders—representing academia, industry, funding agencies, and scholarly publishers—have come together to design and jointly endorse a concise and measurable set of principles that we refer to as the FAIR Data Principles. The intent is that these may act as a guideline for those wishing to enhance the reusability of their data holdings. Distinct from peer initiatives that focus on the human scholar, the FAIR Principles put specific emphasis on enhancing the ability of machines to automatically find and use the data, in addition to supporting its reuse by individuals.

[HTTPS://WWW.NATURE.COM/ARTICLES/SDATA201618#ABS1](https://www.nature.com/articles/sdata201618#ABS1)

The FAIR Guiding Principles

To be Findable:

- F1. (meta)data are assigned a globally unique and persistent identifier
- F2. data are described with rich metadata (defined by R1 below)
- F3. metadata clearly and explicitly include the identifier of the data it describes
- F4. (meta)data are registered or indexed in a searchable resource

To be Accessible:

- A1. (meta)data are retrievable by their identifier using a standardized communications protocol
 - A1.1 the protocol is open, free, and universally implementable
 - A1.2 the protocol allows for an authentication and authorization procedure, where necessary
- A2. metadata are accessible, even when the data are no longer available

To be Interoperable:

- I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
- I2. (meta)data use vocabularies that follow FAIR principles
- I3. (meta)data include qualified references to other (meta)data

To be Reusable:

- R1. meta(data) are richly described with a plurality of accurate and relevant attributes
 - R1.1. (meta)data are released with a clear and accessible data usage license
 - R1.2. (meta)data are associated with detailed provenance
 - R1.3. (meta)data meet domain-relevant community standards

There are an increasing number of resources targeted at supporting the movement to FAIR data, a couple of which are included here to get you started. There is much to cover on this topic, but these links and materials are a start on the conversation.

[How to GO FAIR](#)

[FAIR Implementation Project](#)

References

- NIST:
<https://www.nist.gov/itl/ssd/information-systems-group/configurable-data-curation-system-cdcs/cdcs-help-and-resources-1>
- scientific data (Nature.com): <https://www.nature.com/articles/sdata201618#Abs1>
 - Local link in case above link fails: [The FAIR Guiding Principles for scientific data management and stewardship](#)