Mechanical Testing Ontology for Digital-Twins: a roadmap based on EMMO

Joana Francisco Morgado[1], Emanuele Ghedini[2], Gerhard Goldbeck[3], Adham Hashibon[1], Georg J. Schmitz[4], Jesper Friis[5], and Anne F. de Baas

[1] Fraunhofer Institute for Mechanics of Materials IWM, Germany
[2] Department of Industrial Engineering, University of Bologna, Italy
[3] Goldbeck Consulting Ltd, St. Johns Innovation Centre, Cambridge CB4 0WS, UK
[4] ACCESS, RWTH Aachen University, Germany
[5] Materials and Nanotechnology, SINTEF Industry, Norway

Abstract. The enormous amount of materials data currently generated by high throughput experiments and computations poses a significant challenge in terms of data integration and sharing. A common ontology lays the foundation for solving this issue, enabling semantic interoperability of models, experiments, software and data which is vital for a more rational and efficient development of novel materials. This paper is based on the current efforts by the European Materials Modelling Council (EMMC) on establishing common standards for materials through the European Materials & Modelling Ontology (EMMO) and demonstrates the application of EMMO to the mechanical testing field. The focus of this paper is to outline the approach to develop EMMO compliant domain ontologies.

Keywords: Ontology · Materials Science · Knowledge Base · Digitalisation · Interoperability · EMMO

1 Introduction

Materials Science is a well-established discipline essential to provide new materials that can cope with the current environmental challenges and that can enhance sustainability. The industrial materials development cycle is highly dependent on large volumes of data continuously generated from experiments, characterisation and simulations. Unfortunately, a considerable part of this data ends up unutilised and, in some cases, even discarded leading to loss of opportunities for added value creation. One of the reasons behind this is known as the "silo problem" in data management which basically means a lack of data interconnection and interoperability. This lack hinders full data access and therefore the ability to build new knowledge. The silos are mostly driven by large amount of data being kept in disparate and isolated data sources, heterogeneity of data formats and types and poor curation practices(*e.g.* data from different microstructure modelling generated by commercial software and inhouse codes with no common standards). As reported in a PricewaterhouseCoopers (PwC) study [15], the non-existence of findable, accessible, interoperable and reusable (FAIR) data invokes

Copyright © 2020 for this paper by its authors. Use permitted under Creative Commons License Attribution 4.0 International (CC BY 4.0).

CEUR-WS.org/Vol-2615/paper3.pdf

costs to the European economy of at least €10.2 billion per year and has significant impacts on manufacturing [11].

Digitalisation of materials is playing a vital role in opening data silos and making them exploitable. However, to maximise benefit and to succeed in the digital transformation, all components required to establish a material digital twin must be available [14]. Already existing and mature materials modelling approaches [10] (digital model and data representation) along with the materials data from characterisation and experiments (data from the tangible object: the material) are not sufficient. The information needs also to be formalised and combined [19]. Hence, interoperability of models, software and data is needed to facilitate an integrated approach to materials design and product improvement [9, 22].

Interoperability can be achieved by a common standardised representation of knowledge in the form of an ontology. An ontology consists of a formal, shared, explicit knowledge representation with a common vocabulary which can be used by different people – and machines – to share information within a certain domain and which has interlinked concepts (classes) and individuals (instances) based on a fixed logic formalism (axioms, relationships and subclassification). An ontology is conceptually important to establish a standard or “common language” but also a practical necessity in data knowledge and data management. It provides rich machine processable semantic descriptions that enable complex search terms. An ontology increases the performance of searches [12] in particular as semantic reasoning allows to derive new information using inference and Artificial Intelligence (AI). By leveraging available information, new synergies and knowledge can be produced that can support building better materials, more robust processes and eventually smarter industries and science based on well-informed and well-reasoned decisions.

Attempts to develop ontologies have been made for the materials science field [7, 28, 5, 6]. However, these efforts mostly focus on a specific application and do not always go beyond a taxonomy. Besides an agreed terminology, an ontology requires conceptualisation of logical relations and a set of functional and actionable axioms. To address the interoperability issue, the EMMC has developed the EMMO that provides a common semantic framework for describing materials, models and data with the possibility of extension and adaptation to other domains of interest in the applied sciences. This article is a step towards demonstrating an application of the EMMO to the field of mechanical testing. It is by no means intended to be either complete or to show a complete domain ontology, but rather to show ongoing efforts towards a coherent bottom up and top down ontology development.

2 Methodology

Ongoing efforts to establish a practical ontology for the materials field and in particular for mechanical testing based on the European Materials & Modelling

Ontology (EMMO) are presented within two main sections: EMMO foundations and EMMO domain application development.

2.1 EMMO foundations

EMMO is a top and middle level [20] ontology developed by the EMMC which aims at paving the road for semantic interoperability providing a generic common ground for describing materials, models and data that can be extended to and adapted by all domains of science and engineering. To satisfy the representational needs of the complex and multidisciplinary domain of materials science, EMMO is (i) solidly based in physical sciences, (ii) consistent with fundamental theories such as classical physics and quantum mechanics and (iii) based on existing standards for materials modelling (Review of Materials Modelling [8], CEN Workshop Agreement [1] including the MODA template [2], and other international standards such as the SI Brochure [16] and JCGM200:2008. [3]).

Moreover, to the best of our knowledge, EMMO is the only materials science ontology able to explicitly capture all granularity levels of description of process and materials. These granularity levels can be described in a reductionistic perspective, and this is done via the introduction of the “direct parthood” relation in EMMO. With this relation physicals (the class that contains all the individuals that stand for real world objects that interact physically with the ontologist) [26] can be represented by a strict hierarchy of direct parts down to an elementary level. Direct parthood is a concept in Mereotopology, a combination between mereology and topology used to represent the parthood and spatial-temporal relationships, respectively. EMMO makes extensive use of concepts and relations of mereotopology. Additionally, EMMO has a strong basis in analytical philosophy and relies on causality (physics) and on semiotics. Semiotics reduces the complexity of a physical thing to a sign(model) [9, 22]. The semiotic relationship “standsFor” is the general basis for linking models to reality and this is expressed in the statement “Model standsFor RealThing”. In its formalisation, EMMO is based on *description logic*, and its axiomatisation is expressed using the Web Ontology Language (OWL).

EMMO relies on four main layers: (1) a top level which contains the most fundamental concepts; (2) a middle level that includes representations of generic cross-domain concepts such as materials, units and processes; (3) a domain level for a particular branch of science which is more specialised and specific to concepts and entities relevant within that particular branch of science and engineering; an example is mechanical testing and (4) the application level which should deal only with concepts that are not reused in other applications; an example is concepts specific to a user case such as the name of the measurement device. These layers put into the ontology have to strike a balance between being a highly expressive, (thus heavy) ontology or being a lighter, incomplete but highly efficient ontology. This is the reusability-usability trade-off problem [17].

Especially for measurement processes, having the right unit ontology that addresses the main focus of the community [24], EMMO includes a metrology module at its middle level, used to represent the units and their interlinking with physical quantities. The EMMO with its top and middle level ontology, can be interpreted as the glue combining different domains by providing the root concepts and sockets to plug-in new ontology branches or existing domain and application ontologies.

2.2 EMMO domain application development

The process of ontology development is a thoroughly iterative process with several feedback loops. In fact, it is open-ended since our perception of knowledge changes continuously [19]. Therefore, it is important to adopt a systematic ontology development approach to accompany the knowledge dynamics, capture effectively the complexity of the domains and to follow the ontology stakeholders [4, 13, 21, 23]. EMMO-compliant domain ontologies are developed using the EMMO top and middle level, which gives the advantage of having already a semantic framework in place that provides common standard EMMO concepts as well as established formalized axioms that can be used as root and adapted to the particular purpose.

The presented ontology development methodology follows the common practices in ontology development which consists of the following five phases described by Sure et al. [25]: (1) feasibility study; (2) kickoff; (3) refinement; (4) evaluation and (5) application and evolution.

The development of EMMO domain ontologies starts with the feasibility study, phase (1), which relies on the identification of the domain of interest. The kickoff phase (2) is the most extensive phase and will be the focus of the present paper together with the evaluation phase (4). The former aims at producing the baseline taxonomy which involves the identification of the key terms and concepts to represent the domain of interest in a semi-formal way mostly by the aid of simpler and comprehensive diagrams (*e.g.*: UML or even pen and paper diagrams). In this phase, a classification of the domain based on subclassification relationships (class and subclass) is realized. The conceptualization guided by the EMMO framework should also take place at this stage. It is very important to understand how the main concepts such as process or material are described in EMMO to ensure full compliance of the taxonomy with EMMO notions. EMMO and the domain ontology are then combined by ensuring there is an equivalent EMMO class or suitable EMMO parent class. This consistency in concept enables then an integration between the EMMO and the new domain which starts with the placement of the new concepts as subclass of EMMO classes through a bottom up approach. In the refinement phase (3), the taxonomy hierarchy is formalized using an ontology representation language. In the present paper the ontology is coded using OWL via the open-source ontology editor Protégé [18] and the FaCT++ reasoner [27]. The taxonomy is further enhanced with new concepts (classes) and relations (other than isA) compliant with the EMMO logical constructs are added between the concepts. To comply with the modular design of EMMO a new module (or OWL file) needs to be created per domain which imports not only the EMMO-top and middle level classes and especially EMMO relations but also any other relevant EMMO compliant module and domain.

Usually the evaluation phase is parallel to the refinement due to the need for constant verification and validation with respect to the semantics incorporated, accuracy and completeness [4]. The evaluation (phase 4) of the ontology requires collaboration with both ontology and domain experts which is supported by using the full capabilities of the EMMO open-access GitHub repository [26]. The fifth and last phase, comprising the application and evolution is not addressed within this paper. However, it is important to note that any ontology requires maintenance to be able to respond to the continuous changes in the domain. The maintenance is mostly accomplished by the realization of phases (2)-(4) by the person in charge of gathering and implementing the feedback from the ontology users and applications. A more detailed schematic of the engineering ontology methodology used in the development of EMMO compliant ontologies is represented in Fig. 1. The development steps will be explored further in the following section using the current efforts on the mechanical testing representation as use case.

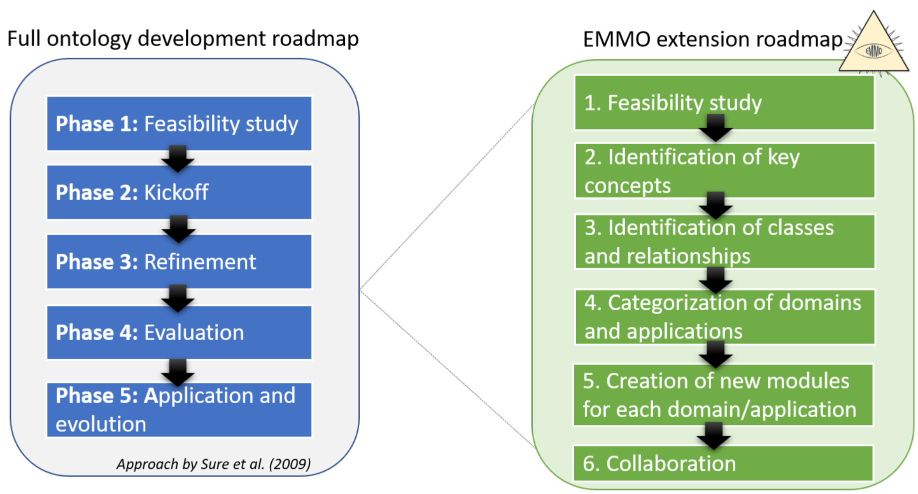

Fig. 1. Overview of EMMO compliant ontologies development steps.

3 Results and Discussion

The main focus of this paper is on how to do the organisation of domain ontologies. We will present the development approach and the discussion of issues related to the identification of commonalities and determination of boundaries between the domains. Ongoing efforts on the mechanical testing EMMO-compliant domain ontology are presented as an example.

Mechanical testing covers a wide range of tests that are carried out to determine the mechanical properties of materials. The purpose is to ensure that their material response to a given action makes the material suitable for the intended application. The methodology for formalising this domain in an EMMO compliant ontology is carried out following the six main steps identified in the green (right) part of Fig. 1

1. Feasibility study: The domain of interest of this paper is mechanical testing.

2. To satisfy the aim of the ontology, the semantic model should support the representation of a process that can be used to represent the mechanical tests and the material defined by its properties before,during and after the tests. This is shown in Fig. 2.

3. Identification of classes and relationships: Based on the main concepts of process, material and properties the initial ontology structure as represented in Fig. 2 can be built and is further enhanced by the addition of new classes and EMMO-compliant logic constructs.

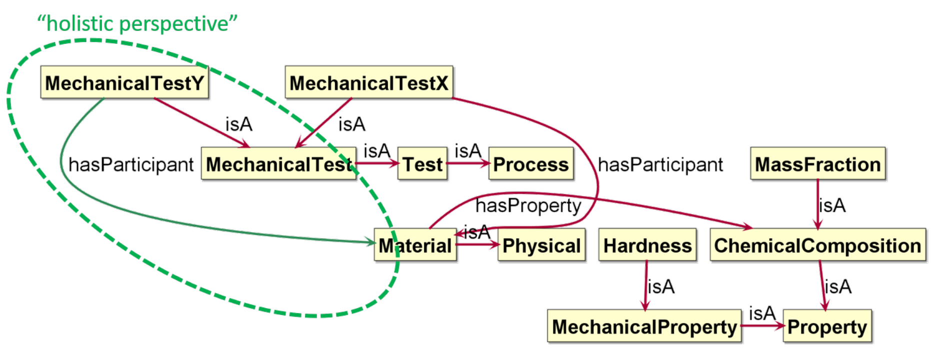

Fig. 2. Excerpt of the initial concept diagram for the mechanical testing classes and EMMO "holistic perspective".

Each object and relation is discussed and it is determined to which EMMO perspective it belongs (holistic, physics or reductionistic. e.g. hasParticipant and hasRole are emmo-relationships specific to physicals represented in an "holistic perspective" that focusses on the role of the participants Fig. 2.
The formalisation of the classes and relationships in OWL is realised in parallel together with the constant verification of the ontology consistency. This is the key step in the ontology development procedure since it maps the real-world entities/objects with their ontological representations.
Note that to achieve completeness, the developed ontology should just contain enough concepts, classes and relationships to respond to the desired competency questions.

4. Categorization of domains and applications: The level of genericness of each concept needs to be discussed and it needs to be decided whether the concept belongs to a domain or an application level. The class MechanicalTestX that represents a specific type of mechanical test is application-specific knowledge and it is a subclass of the domain notion MechanicalTest (Fig. 2). Please note that this is true because the MechanicalTestX class refers here to a variant of a mechanical test (*e.g.*: tensile test or indentation test part of the domain level) that is specific to a certain Lab X. More general concepts such as the classes properties, process and material are part of the EMMO middle level.

5. Creation of new modules for each domain/application: EMMO compliant ontologies are sliced in several modules which are used to separate domain and application-specific knowledge. This ensures the design of a modular ontology which facilitates its progress and gradual enrichment. Fig. 3 shows an example of three modules that need to be developed to represent the mechanical test: mechanical-test-x, mechanical-test-y and mechanical-testing. The modules mechanical-test-x, mechanical-test-y are part of the application layer and contain concepts that are specific to each of these tests (not shared among them) *e.g.* the name of the operator or name of the measurement device whereas the module mechanical testing, which is part of the EMMO domain layer contains more generic concepts that are used in both mechanical-test-x and mechanical-test-y modules. Concepts represented in Fig. 3 other than MechanicalTestX, MechanicalTestY and MechanicalTest are part of other modules at the middle and top levels of EMMO. It is worth mentioning that the practice is adopted to make each of this modules correspond to an OWL file with a specific namespace *e.g.*“http://emmo.info/emmo/application/mechanical-test-x”.

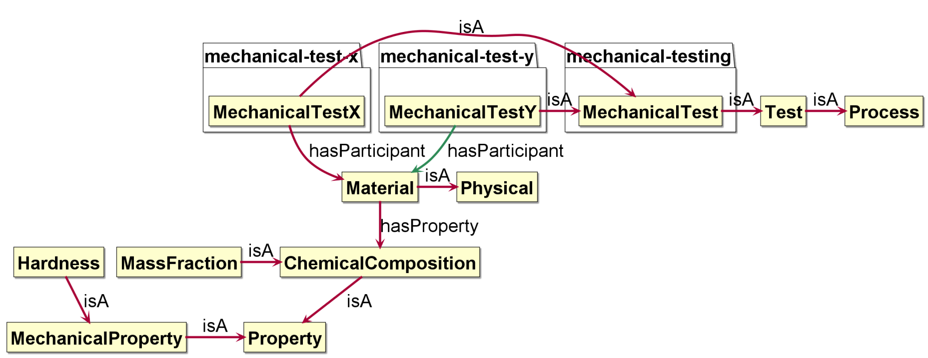

Fig. 3. Representation of some of the modules developed for mechanical testing.

To get the domain/application ontologies accepted as an ontology based on EMMO using the official EMMO repository, the end-user needs to submit a proposal to the EMMO Governance Committee. Once approved, a Domain Ontology Task Group will be established by the EMMC for the maintenance and development of the designated ontology.

The integration of these modules and the placement in the different emmo levels (top, middle, domain and application) is represented in Fig. 4 where the yellow rectangle represents the top and middle layers (core framework) that are the building block for all EMMO compliant ontologies. This work was based on the currently available EMMO v1.0.0-alpha2 version on GitHub.com.

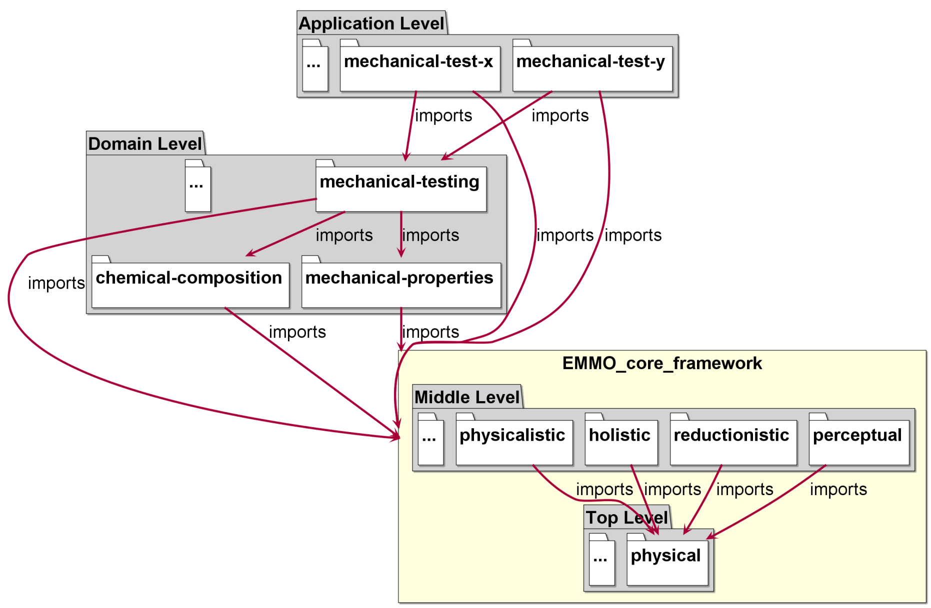

Fig. 4. Modular framework of EMMO compliant ontologies.

6. Collaboration: The development of a harmonious, coherent, common standard in an application field is achieved by using the emmo top and middle level ontology and by engaging the whole mechanical testing stakeholder community from material science, industry and research in its development. Hence, to ensure the participation of all interested communities, this application domain ontology is open-source and relies on its open-access repository in GitHub for development [26].

4 Conclusion

This paper supports the current Industry 4.0 efforts to move towards integrated knowledge. The paper presents EMMO as a basis to document material science by establishing a ontology engineering methodology and demonstrating this via an application of EMMO in the field of mechanical testing . The presented building blocks are vital to bridge the gap between the modern experimental, simulation and characterisation fields. The presented integration is shown to result into actionable knowledge that can support intelligent and well-informed decision-making along development of novel materials solutions.

5 Acknowledgements

This paper is supported by European Union's Horizon 2020 research and innovation programme: MARKETPLACE project, Grant Agreement No. 814492; FORCE project, Grant Agreement No. 721027 and OYSTER project, Grant Agreement No. 760287.

References

1. CEN workshop agreement - CWA 17284 - materials modelling - terminology, classification and metadata. https://ftp.cencenelec.eu/CEN/TCandWorkshops/Workshops/WS/%20MODA/CWA 17284.pdf, 04-03-2020
2. MODA template. https://moda-app.eu/, 04-03-2020
3. 200:2008, J.: International vocabulary of metrology — basic and general concepts and associated terms (2008)
4. Ameri, F., Urbanovsky, C., McArthur, C.: A systematic approach to developing ontologies for manufacturing service modeling. In: Proceedings of the workshop on ontology and semantic web for manufacturing. vol. 14. Citeseer (2012)
5. Ashino, T.: Materials ontology: An infrastructure for exchanging materials information and knowledge. Data Science Journal (2010)
6. Bhat, M., Shah, S., Das, P., Kumar, P., Kulkarni, N., Ghaisas, S.S., Reddy, S.S.: Premap- knowledge driven design of materials and engineering process. In: ICoRD'13 (2013)
7. Cheung, K., Drennan, J., Hunter, J.: Towards an ontology for data-driven discovery of new materials. In: AAAI Spring Symposium: Semantic Scientic Knowledge Integration (2008)
8. De Baas, A.: What makes a material function. Let Me Compute the Ways... Modelling in H2020 LEIT-NMBP Programme Materials and Nanotechnology Projects. Luxembourg: Publications Office of the European Union (2017)
9. Goldbeck, G., Ghedini, E., Hashibon, A., Schmitz, G.J., Friis, J.: A reference language and ontology for materials modelling and interoperability. In: Proceedings NAFEMS World Congress (2019)
10. Goldbeck, G., Court, C.: The economic impact of materials modelling (Jan 2016). https://doi.org/10.5281/zenodo.44780, https://doi.org/10.5281/zenodo.44780

11. Goldbeck, G., Simperler, A.: Strategies for industry to engage in materials modelling (Dec 2019). https://doi.org/10.5281/zenodo.3564455, https://doi.org/10.5281/zenodo.3564455
12. Himanen, L., Geurts, A., Foster, A.S., Rinke, P.: Data-driven materials science: Status, challenges, and perspectives. Advanced Science **6**(21), 1900808 (2019)
13. Järvenpää, E., Siltala, N., Hylli, O., Lanz, M.: The development of an ontology for describing the capabilities of manufacturing resources. Journal of Intelligent Manufacturing **30**(2), 959–978 (2019)
14. Kritzinger, W., Karner, M., Traar, G., Henjes, J., Sihn, W.: Digital twin in manufacturing: A categorical literature review and classification. IFAC-PapersOnLine **51**(11), 1016–1022 (2018)
15. Lahmann, M., Probst, M., Parlitz, T.: Benefits management - transformation assurance. Tech. rep. (2019)
16. des Poids et Mesures, B.I.: The international system of units (si) (2019)
17. Morbach, J., Yang, A., Marquardt, W.: Ontocape—a large-scale ontology for chemical process engineering. Engineering applications of artificial intelligence **20**(2), 147–161 (2007)
18. Musen, M.A.: The protégé project: a look back and a look forward. AI matters **1**(4), 4–12 (2015)
19. Ocker, F., Paredis, C.J., Vogel-Heuser, B.: Applying knowledge bases to make factories smarter. at-Automatisierungstechnik **67**(6), 504–517 (2019)
20. Rudnicki, R., Smith, B., Malyuta, T., Mandrick, W.: Best Practices of Ontology Development (2016)
21. Sack, H.: Knowledge engineering with semantic web technologies. https://open.hpi.de/courses/semanticweb2015, 04-03-2020
22. Schmitz, G.J., Goldbeck, G., Ghedini, E., Hashibon, A., Friis, J.: Towards an icme methodology in europe – nomenclature, taxonomies, ontologies, and marketplaces. In: Proceedings NAFEMS World Congress (2019)
23. Staab, S., Studer, R.: Handbook on Ontologies. Springer (2009)
24. Steinberg, M.D., Schindler, S., Keil, J.M.: Owl: Experiences and directions–reasoner evaluation. OWL: Experiences and Directions–Reasoner Evaluation. (2016)
25. Sure, Y., Staab, S., Studer, R.: Ontology engineering methodology. In: Handbook on ontologies, pp. 135–152. Springer (2009)
26. EMMO: European Materials and Modelling Ontology (EMMO) repository template. https://github.com/emmo-repo/EMMO, 04-03-2020
27. FaCT: The FaCT system. http://www.cs.man.ac.uk/ horrocks/FaCT/, 04-03-2020
28. Zhang, X., Hu, C., Li, H.: Semantic query on materials data based on mapping matml to an owl ontology. Data Science Journal (2009)