


Agile Research Data Management with Open Source: CaosDB

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Software can be found here: <https://gitlab.com/caosdb>
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Abstract.

Research data management (RDM) in academic scientific environments increasingly enters the focus as an important part of good scientific practice and as a topic with big potentials for saving time and money. Nevertheless, there is a shortage of appropriate tools, which fulfill the specific requirements in scientific research. We identified where the requirements in science deviate from other fields and proposed a list of features which RDM software should fulfill to become a viable option.

Finally we analyzed the open-source RDMS CaosDB for compatibility with the proposed features and found that it fulfills the requirements.

1 **1 Introduction**

2 Research units, from small research groups at universities to large research and development
3 departments are increasingly confronted with the challenge to manage large amounts of data, data
4 of high complexity[1], [2] and changing data structures[3], [4]. The necessary tasks for research
5 data management include storage, findability and long-term accessibility for new generations of
6 researchers and for new research questions[4]–[6].

7 In spite of the advantages of implementing data management solutions[7], there is a lack of
8 standard methods or even standard software so far for research data management, especially
9 in the context of quickly evolving methods and research targets. In this article, we define the
10 specific challenges for research data management (RDM) and propose features which suitable
11 RDM software should have to (a) fulfill the practical needs and (b) be accepted by the potential
12 users. We also demonstrate how the CaosDB¹[8] toolkit is a viable approach to satisfy all the
13 proposed requirements.

1. Website: <https://caosdb.org>, source code: <https://gitlab.com/caosdb/>

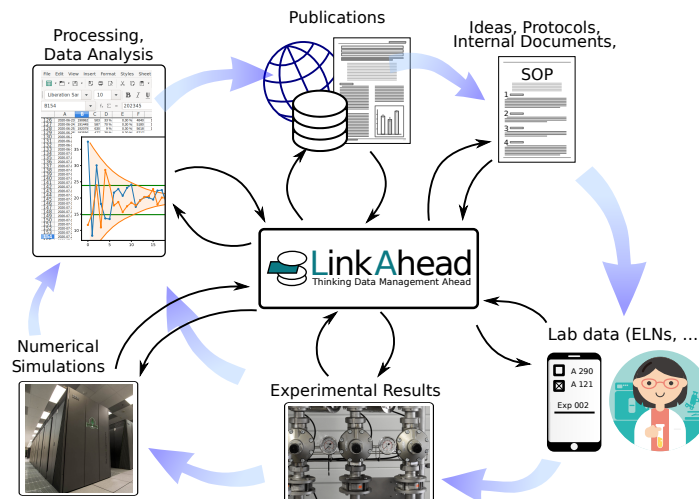


Figure 1: Schematic illustration of the scientific data lifecycle. Data can be obtained from every step, and in most cases the relationship between data entities is just as relevant as the raw data. While this example focuses on experimental and laboratory centered disciplines, comparative lifecycles also exist for theoretical sciences and most fields in the humanities.

14 2 Challenges for research data management

15 2.1 The scientific data lifecycle

16 Data which accrues in scientific research is more than just experimental readings, field notes
 17 or interview recordings. In order to fully represent the research journey and eventually enable
 18 reproducible science, the data from every research step may become relevant and thus should be
 19 consistently managed.

20 Figure 1 shows a schematic of different research steps during the research lifecycle, during which
 21 important data is generated. For full reproducibility, it is not sufficient however to simply store
 22 the data acquired at each point, but also to represent the semantic connections and make them
 23 searchable.

24 In more detail, the most relevant data source in scientific research are:

25 **Prior publications** An important part of good scientific practice (GSP) is to credit the influence
 26 of prior work, by the scientists themselves or third parties. Linking one’s work to previous
 27 publications and making these connections public also helps to assess reproducibility and
 28 may lead to fruitful data-reuse in unforeseen contexts.

29 **Ideas and SOPs** The data here consists mostly of text documents which describe thoughts,
 30 hypotheses and planned standard operating procedures (SOPs). These documents fill the
 31 gap between previous work and the next round of data acquisitions, they often also work
 32 as a blueprint for the data acquisition phase.

33 **Lab data** Environmental data, device settings, used SOPs and ingredients and other incidental
 34 data typically accrues during the course of experiments and was traditionally stored in paper
 35 laboratory notebooks. Currently, a lot of laboratories switch to electronic lab notebooks
 36 (ELNs) for the same purpose. While this data is often seen as second-class “metadata”,

37 we hold that since often conclusions can be drawn from it, it deserves the same handling
38 as final instrument readings.

39 **Experimental results** These are what is often considered the *main* data. For analysis, it mostly
40 still needs parameters from at least the previous step, to filter for special conditions, to
41 compare settings or to verify that values are compatible with standard literature.

42 **Numerical simulations** Similarly to experimental results, data obtained from numerical meth-
43 ods can not be interpreted without knowledge about used software and parameters, possibly
44 hardware conditions and input from laboratories or third-party data sources. Since bit-exact
45 reproducibility is possible in theory, all relevant settings should be stored unchanged.

46 **Data analysis** When analyzing data from previous steps, storing not only the used programs,
47 scripts and their parameters, but also the semantic connections enables later researchers
48 to reconstruct which method was used, which assumptions were made and under which
49 conditions the input data was gathered.

50 **Next publication** Formally the end of the lifecycle, but of course also the beginning of many
51 new ones, a publication contains a number of statements which are supported by data
52 from previous steps. A comprehensive research RDM system (RDMS) could quickly
53 summarize, for each plot in a publication, how the data was analyzed and acquired and
54 under which assumptions the experimental setting was planned.

55 This list focuses on experimental and laboratory centered disciplines, but of course in the
56 humanities and theoretical sciences, there are equivalent steps which are equally important to
57 preserve and link to each other.

58 2.2 Specifics of scientific research data management

59 Existing data management systems (DMS) often still follow the paradigms of relational databases[9],
60 [10]: There is a number of types for the data, with each type having a number of possible proper-
61 ties. Each stored entity belongs to one type and has the properties defined by the type, occasionally
62 it is also possible to leave a property empty or *undefined*. Searching or filtering in the stored data
63 entities is possible by criteria which operate on the content of the properties and on the data types.
64 These DMS have been widely successful in many areas such as finance, administration and
65 high-tech industries[11], [12], but remain scarce in both academic and private sector research[12],
66 [13].

67 We hold that the main reasons are:

68 **Interoperability** Scientists tend to work with their own custom-written software, which often
69 requires files with data to be directly accessible to the OS via a – remote or local – file
70 system. Many DMS store data files internally and make them available only via download.
71 Also programmatic access (query, retrieve, update) to data DMS solutions via network
72 APIs was uncommon until a few years ago, so that acquired data could not be instantly
73 integrated in the DMS.

74 **Agility** Traditional DMS require users to define a data model and stick to it. All data to be
75 entered has to conform to the data model as it was defined. Research however is defined

76 by having undefined outcomes, the research questions, experimental setup or analysis
77 methods change more often than not over the course of one investigation. A DMS based
78 on rigid SQL databases thus may soon become a liability instead of an asset.

79 **Learning curve** Research is impossible without the contribution of many participants, with
80 different qualifications. With many DMS, it takes a lot of active learning before users can
81 benefit from the provided data.

82 **Practical use** Systems which only store data, but do not provide short-term advantages, have
83 high entrance barriers everywhere. In academic research however, junior scientists with
84 short-term contracts have little incentive to invest time and money in systems which only
85 may pay out on longer timescales.

86 3 Proposed features

87 Under the assumptions from the previous sections, we propose the following core properties
88 which an RDMS should have:

89 **Semantic linkage** To fully map the real-world environment of data entities to the RDMS, it
90 must be possible to link data sets with each other in a meaningful way. The default linking
91 possibilities and properties of the data types in the RDMS form the *data model*.

92 **Deep search** The RDMS should have easily accessible search options not only for property
93 values of stored entities, but also for links to other entities and properties (and link) thereof.

94 **Flexible data model** Researchers require an RDMS where the data model can be changed on
95 the fly, without the need to migrate or discard existing data. When the data model is
96 changed, for example due to new machines, protocols or evolving research questions, the
97 existing data must remain valid and usable.

98 **Versioning** Mistakes during data acquisition happen, and it must be possible to correct existing
99 data sets. At the same time, this editing must be made transparent and the history of each
100 data set must be kept for future inspection.

101 **File system integration** For interaction with third-party programs, raw data files must be avail-
102 able on standard file systems. Ideally the scientists' workflows should remain unchanged
103 by the RDMS.

104 **Open APIs** For machine interaction with third-party programs, the RDM must have a well-
105 documented API. In research contexts, these programs are often custom-written by scien-
106 tists without explicit computer science background, so extensive documentation is very
107 desirable.

108 3.1 User acceptance

109 Additionally, to increase the acceptance by potential users, we focus on two additional areas,
110 automated data integration and low-threshold search options.

111 3.1.1 Automation

112 Automation of repetitive data integration reduces error rates and frees users to concentrate on
113 more challenging tasks. It is therefore desirable for an RDMS to have:

114 **Synchronization** The RDMS should make it easy for its administrators to integrate existing
115 data sources (for example databases or file systems with structured folder hierarchies)
116 into the RDMS: The RDMS should be synchronized automatically with data from these
117 sources, which makes these data available in a unified manner via the RDMS interface.
118 Note that the RDMS can not solve the conceptual problem of a single source of truth when
119 synchronizing data from different sources, but it can at least highlight potential conflicts
120 and where they first occurred to administrators.

121 **ELN integration** Research work in the lab is increasingly documented with electronic lab
122 notebooks (ELNs)[14], [15], which allow to conveniently enter device and experimental
123 settings in a semi-structured way. This data is usually critical in the analysis of acquired
124 raw data from instruments, e.g. for searching specific data sets or filtering by parameters.
125 There should be a possibility that the RDMS integrates the ELN data and presents it like
126 data from other sources.

127 **Workflow representation** While following one SOP, the laboratory workflow is often highly
128 standardized, which makes it suitable for representation within the RDMS. The RDMS
129 should support workflows with different states, which can only be switched in an admin-
130 defined pattern. This simplifies the work for users, because they may e.g. only see the
131 interfaces which are relevant for the current sample processing step.

132 3.1.2 Simplified search

133 To overcome initial reluctance by users, it is important to flatten the learning curve[16]. Besides
134 obvious requirements such as user-friendly documentation, we hold that it is especially important
135 to provide simplified search options. The simplified search in an RDMS should give some early
136 sense of achievement, so users can understand that an RDMS will lead to a simplification of
137 their work.

138 4 CaosDB

139 We hold that CaosDB[8], a flexible data management framework, fulfills the above-mentioned
140 requirements. CaosDB was initially developed by one of our colleagues, Timm Fitschen, during
141 his time at the Max Planck Institute for Dynamics and Self-Organization. In 2018, CaosDB was
142 released under the AGPLv3 license on [gitlab.com](https://gitlab.com/2)². Since 2020, CaosDB has found increased
143 adoption in multiple research facilities.

144 4.1 Data Model

145 CaosDB's *meta* data model is shown schematically in Figure 2. The base type for everything
146 is ENTITY, with the inheriting types PROPERTY (attributes of ENTITIES, may be list values and

2. <https://gitlab.com/2>

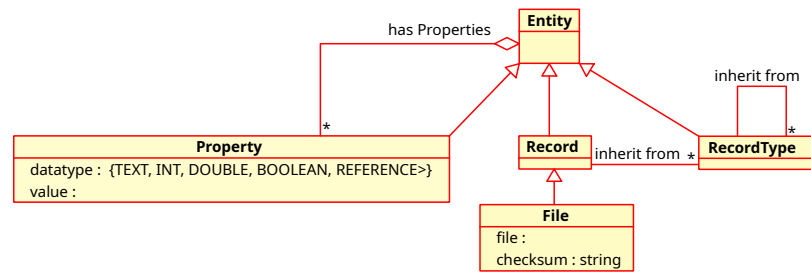


Figure 2: The meta data model of CaosDB.

147 references to other ENTITIES), RECORDTYPE (templates for actual data sets) and RECORD. Actual
 148 data is typically stored in RECORDS, which *inherit* from one or more RECORDTYPES and thus
 149 have all the PROPERTIES defined therein. The RECORDTYPES may form a complex inheritance
 150 hierarchy themselves. FILE entities are similar to Records, but additionally are connected to
 151 files which may reside on conventional file systems or potentially in abstracted cloud storages.
 152 This approach to use files at their current locations instead of duplicating file content not only
 153 increases CaosDB’s scalability, but also lower the entrance barrier, since scientists can access
 154 the managed file in their traditional ways.

155 Details of this meta data model in CaosDB are elaborated on in [8], but it should be clear now
 156 already that CaosDB provides the *Semantic linkage* feature.

157 In CaosDB, the *data model* of the stored data refers to the RECORDTYPES and their PROPERTIES,
 158 which together describe the pattern to which newly created data sets should conform. The data
 159 model in CaosDB can be modified at any time, but the changes only take effect for data to
 160 be inserted *after* this modification. Existing data is not affected and remains unchanged. This
 161 property fulfills the proposed *Flexible data model* feature.

162 This possibility to completely change the data model, while not giving up on a general structure,
 163 places CaosDB between traditional SQL based relational databases and NoSQL³ approaches (c.f.
 164 Figure 3). While we described above why rigid SQL databases are not suited for use in dynamic
 165 research environments, giving no structure (the NoSQL paradigm) tends to lead to incoherent
 166 data which is hard to search⁴. A third approach, using graph databases to represent semantic
 167 information, has not found its way into general adoption to our knowledge, presumably because
 168 the query languages tend to become very unwieldy, compare the appendix 7 for an example.

169 4.2 Architecture and Libraries

170 CaosDB uses a client/server based architecture, as depicted in Figure 4a. CaosDB has is a REST
 171 API for simple access by traditional clients and a web interface for browsers, as well as a gRPC
 172 API which allows for more complex operations, such as atomic content manipulations. The
 173 existing client libraries⁵ and the open APIs provide the proposed *Interoperability* requirement.

174 One particularly useful client library component is the *CaosDB Crawler* framework. This
 175 extensible framework simplifies the work to synchronize external data sources with CaosDB

3. Popular examples for NoSQL database systems are CouchDB or MongoDB.

4. Missing structure in Data Lakes has lead to the tongue-in-cheek colloquialism “Data Swamp”.

5. A list of the available libraries with the respective source code repositories are given in the Appendix section 6.2.

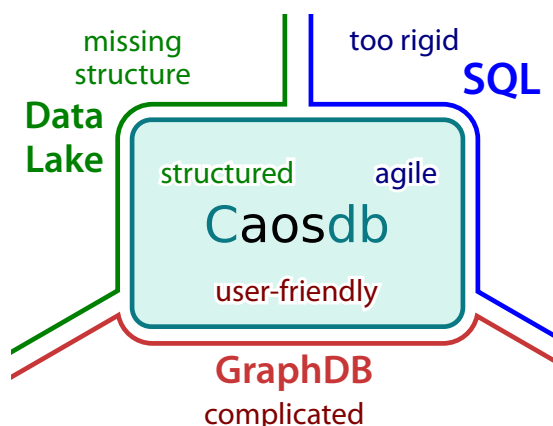


Figure 3: CaosDB compared to other database approaches.

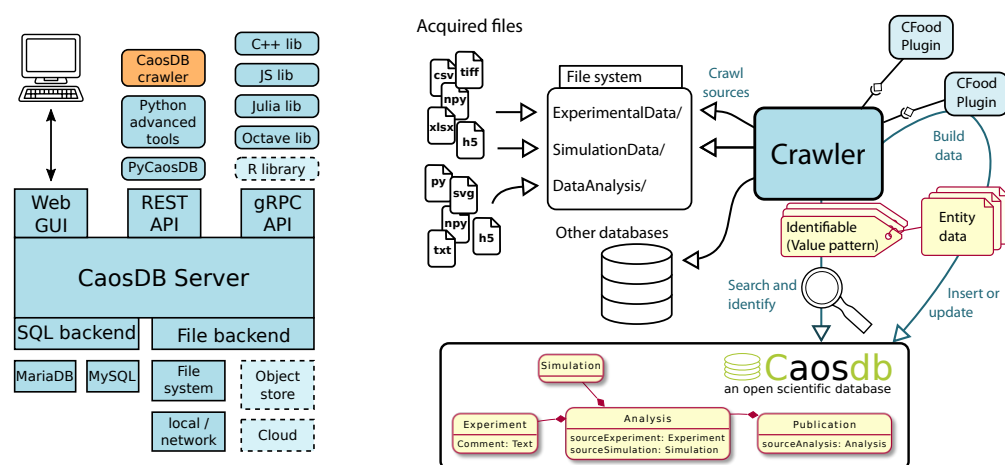


Figure 4: (a) CaosDB's server-client architecture with client libraries and backend components. Dotted elements are under development. (b) The crawler framework facilitates fast development of custom data integration from a diversity of sources.

176 through a plugin system. The crawler workflow can be characterized as follows:

- 177 1. The crawler periodically checks its data sources for new or changed data stores, such as
178 file systems or the content of other databases.
- 179 2. Each new data source is fed to a so-called *CFood plugin* for consumption. There is a
180 choice of existing plugins, or administrators can write their own. The *CFood plugin*'s job
181 is to build CaosDB entities from the consumed data and to specify *Identifiables*, which
182 work as search patterns.
- 183 3. The crawler checks for each *Identifiable* if a corresponding entity exists already in CaosDB.
184 If there is no corresponding entity, the entity as returned by the *CFood plugin* is inserted
185 into CaosDB. If there is already an existing entity, the Crawler will attempt to merge the
186 existing with the new entity and notify the data curators in case of merge conflicts.

187 This tool set provides the *Synchronization* requirement, and if ELNs are used as external data
188 source, the *ELN integration*. Practical use of CaosDB crawler framework has previously been

189 demonstrated in [17] and ELN integration was implemented in [18].

190 4.3 Additional features

191 **Deep search** CaosDB offers a simple semantic query language, which borrows some semantics
192 from SQL, but has a focus on usability for non-technical users. The CaosDB query
193 language makes deep search easy with expressions like the following:

```
194 FIND Analysis WITH quality_factor > 0.5  
195         AND WITH Sample WITH weight < 80g
```

196 This convenient nesting of query expressions circumvents the JOIN operations from
197 traditional SQL languages. A full documentation of CaosDB's query language is available
198 online⁶ or in CaosDB's sources.

199 **Search templates** CaosDB's web interface provides customizable search templates which allow
200 more advanced users to create their own templated queries, which can then be shared with
201 novice users for *simplified searches*. In templated queries, users can insert custom strings
202 into pre-defined locations of a search query, see Figure 5.

203 **Versioning** When entities are modified in CaosDB, time and user of the change are recorded
204 and CaosDB puts the previous version onto a history stack and amends the current version
205 with link to the previous version. Over time, each entity may thus grow to a tree of linked
206 versions, which can be retrieved via the web UI or programmatically through the APIs.
207 This feature of CaosDB enables scientific research data management users to adhere to
208 the principles of good scientific practice.

209 **State management** In CaosDB, users may declare a state machine of states and allowed transi-
210 tions. Users may then affix states to entities, and these states can then only be changed
211 according to the rules of the state machine. In this way, users can implement a *workflow*
212 *representation* which ensure that for example laboratory samples run through a specified
213 list of preparation steps in order.

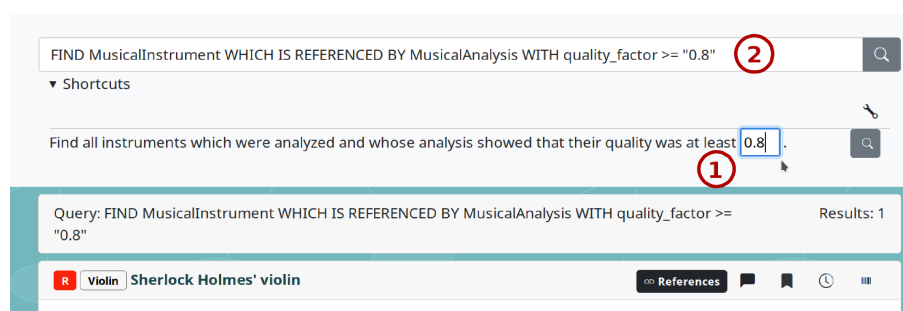


Figure 5: A query template in CaosDB's web UI. The user can enter a custom value into an input field ① and the template is then executed as a plain CaosDB query ②. Screenshot from <https://demo.indiscale.com>.

6. <https://docs.indiscale.com/caosdb-server/CaosDB-Query-Language.html>

214 4.4 Availability and documentation

215 CaosDB is available on the public Git repository gitlab.com at <https://gitlab.com/caosdb>,
216 a detailed list of CaosDB's sub projects is given in the annex.

217 For the interested public, there is a live demo server at <https://demo.indiscale.com>, hosted
218 by IndiScale GmbH. This demo server is actually running LinkAhead, a commercially supported
219 distribution of CaosDB.

220 There are also Debian/Ubuntu packages to run precompiled LinkAhead/CaosDB for download
221 at <https://indiscale.com/download>.

222 CaosDB's sub projects each have their own documentation in their source directories. The
223 documentation is also available online at <https://docs.indiscale.com>.

224 5 Conclusion

225 We found that scientific research has specific requirements to data management: Interoperability,
226 agility, adequate learning curves and early practical use. Most data management system do not
227 satisfy these requirements, so we set up a specific list of features which a scientific RDMS should
228 have. The open source research data management framework CaosDB has the specified features
229 and thus fulfills the requirements for a scientific RDMS.

230 Special attention has to be given to the aspect of synchronizing data from external sources (e.g.,
231 crawled files, ELNs) and records in the RDMS. Different sources can (usually by some error)
232 have conflicting data, or entries in the RDMS can be changed manually by users after their
233 insertion. In our experience, this problem can not be solved in a general and purely technical way.
234 Instead, best practices have to be implemented as to where possible errors should be corrected
235 and whether some sources have precedence above each other. A RDMS like CaosDB, together
236 with the crawler framework, can help administrators identify inconsistencies in the case of two or
237 more data sources. Through versioning, it is visible who and when maybe changed data manually.
238 How to optimize the help in recognizing potential conflicts, and in the end curate data both in
239 the RDMS and in the external sources, is subject of the authors' ongoing research.

240 We hope that the open source license of CaosDB will inspire scientists to contribute to CaosDB.

241 6 Appendix: Software

242 6.1 CaosDB

243 The caosDB suite with the main libraries is published at Zenodo:
244 <https://zenodo.org/record/7752417> (DOI:10.5281/zenodo.7752417)

245 6.2 List of CaosDB libraries

246 The following libraries for programming client applications are publicly available:

247 **Python** <https://gitlab.com/caosdb/caosdb-pylib> The Python client library can be
248 used for third-party applications and is the foundation for several other libraries:

- 249 **Advanced Python tools** <https://gitlab.com/caosdb/caosdb-advanced-user-t>
 250 ools Additional high-level tools, including a legacy implementation of the CaosDB
 251 crawler.
- 252 **Crawler** <https://gitlab.com/caosdb/caosdb-crawler> A new implementation of
 253 the CaosDB crawler.
- 254 **JavaScript** <https://gitlab.com/caosdb/caosdb-webui> The JavaScript library is part of
 255 the web user interface component.
- 256 **Protobuf API** <https://gitlab.com/caosdb/caosdb-protobuf> The gRPC API is defined via
 257 these protobuf files.
- 258 **C++** <https://gitlab.com/caosdb/caosdb-cpplib> The C++ library uses the gRPC API
 259 of CaosDB.
- 260 **Octave** <https://gitlab.com/caosdb/caosdb-octavelib> The Octave/Matlab library is
 261 based upon the C++ library.
- 262 **Julia** <https://gitlab.com/caosdb/caosdb-julialib> The Julia library also is based upon
 263 the C++ library.

264 7 Appendix: Query language comparison

265 As an example for nested queries in different query languages, we consider the search for female
 266 UK-based writers in a certain time period, whose given or family name starts with the letter
 267 M. We used the RDF query language SPARQL with Wikidata⁷ identifiers and CaosDB's query
 268 language with fictional but plausible identifier names.

269 The SPARQL query is as follows:

```


270 SELECT DISTINCT ?item ?itemLabel ?givenName ?familyName WHERE {
271     ?item wdt:P31 wd:Q5; # Any instance of a human.
272         wdt:P27 wd:Q145; # United Kingdom
273         wdt:P21 wd:Q6581072; # female
274         wdt:P106 wd:Q36180; # writer
275         wdt:P569 ?birthday;
276         wdt:P570 ?diedon;
277         wdt:P734 [rdfs:label ?familyName];
278         wdt:P735 [rdfs:label ?givenName].
279     FILTER(?birthday > "1870-01-01"^^xsd:dateTime
280           && ?diedon < "1950-01-01"^^xsd:dateTime)
281     FILTER(regex(?givenName, "M.*") || regex(?familyName, "M.*"))
282     SERVICE wikibase:label { bd:serviceParam wikibase:language "en" }
283 }
```

284 In contrast, the CaosDB query looks like this:

7. <https://www.wikidata.org>

```
285 SELECT given_name, family_name FROM Writer
286 WITH gender=f AND country=UK AND birthday > 1870 AND death < 1950
287 AND (given_name LIKE "M*" OR family_name LIKE "M*")
```

288 8 Acknowledgements

289 We acknowledge the previous work on the CaosDB software by its the main authors and inde-
290 pendent contributors, especially Timm Fitschen .

291 9 Conflicts of interest

292 The authors work for IndiScale GmbH, which provides commercial support and other services for
293 CaosDB and the derived free and open-source LinkAhead distribution. DH and FS contributed
294 to the development of CaosDB.

295 10 Roles and contributions

296 **Daniel Hornung:** Conceptualization, Visualization, Writing – original draft

297 **Florian Spreckelsen:** Conceptualization, Writing – review & editing

298 **Thomas Weiß:** Conceptualization, Visualization

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