

A practical approach to constructing a knowledge graph for soil ecological research

Nicolas Le Guillarme, Wilfried Thuiller

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1 A Practical Approach to Constructing a Knowledge Graph for

2 Soil Ecological Research

3 List of authors: Nicolas Le Guillarme, Wilfried Thuiller

4 Affiliations:

- 5 Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, LECA, F-38000 Grenoble, France.
- 6 Corresponding author: Nicolas Le Guillarme; nicolas.leguillarme@univ-grenoble-alpes.fr

7 Abstract

8 With the rapid accumulation of biodiversity data, data integration has emerged as a hot topic 9 in soil ecology. Data integration has indeed the potential to advance our knowledge of global 10 patterns in soil biodiversity by facilitating large-scale meta-analytical studies of soil 11 ecosystems. However, ecologists are still poorly equipped when it comes to integrating 12 disparate datasets. In recent years, knowledge graphs have emerged as a powerful tool for 13 integrating large amounts of distributed heterogeneous data while making these data more 14 easily interpretable by humans and computers. This paper presents a practical approach to 15 constructing a biodiversity knowledge graph from heterogeneous and distributed 16 (semi-)structured data sources. To illustrate our approach, we integrate several datasets on 17 the trophic ecology of soil organisms into a trophic knowledge graph and show how both 18 explicit and implicit information can be retrieved from the graph to support multi-trophic 19 studies.

20

21 Keywords: data integration, knowledge graph, ontology, reasoning, soil ecology

1

22 Introduction

23 In recent years, a number of initiatives aiming at collecting new soil biodiversity data or 24 assembling existing datasets have emerged, resulting in a rapid accumulation of data in soil 25 ecology [1]. Because of the enormous phylogenetic, taxonomic and functional diversity of 26 soil organisms, datasets are often collected by individual scientists or small project teams 27 from different communities or disciplines to answer precise research questions. These 28 datasets are typically small, with a limited spatial/temporal/taxonomic coverage, and are 29 formatted according to the project needs, with little or no concern for data standardization 30 [2]. This causes datasets to be heterogeneous in semantics (differences in terminologies, 31 meaning or interpretation of data in different disciplines or research contexts), schema 32 (differences in data structures and formats) and syntax (differences in models or languages). 33 In addition, datasets are widely distributed: they reside on diverse locations, e.g. files or 34 databases on the local network or published on the web, and are accessible using different 35 interfaces, e.g., files downloads, database queries or web APIs.

36 Integrating these 'long-tail data' dispersed across different datasets could help address 37 research questions at larger scales [3]. Data integration is of growing interest in the 38 ecological domain, with much effort directed towards the creation of standard terminologies 39 for describing, sharing and facilitating the aggregation of biodiversity data, e.g. organismal 40 trait data [4, 5, 6, 7], into large open databases. Recent initiatives in trait-based ecology have 41 targeted specific taxonomic groups, e.g. ants [8], spiders [9], soil invertebrates [10, 11], fungi 42 [12, 13], plants [14]. Although these databases have made aggregated data more readily 43 accessible to scientists, they are not yet interoperable. The difficulty of integrating data 44 distributed across heterogeneous sources remains. As a result, integrative analyses of soil 45 communities that span several taxonomic groups and integrate multitrophic interactions are 46 scarce — see [15] for an example — although essential to improve our understanding of the 47 links between soil biodiversity and ecosystem functioning [16].

2



49 Figure 1. Semantic data integration provides the user with a uniform access to a set of 50 autonomous and possibly heterogeneous data sources in a particular application domain.

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52 Here, we address the problem of semantic data integration in the biodiversity science 53 domain. Data integration is defined in [17] as the process of combining data residing at 54 different sources, and providing the user with a unified view of these data. (Figure 1). As a 55 result, the user has the ability to seamlessly manipulate data from multiple sources, 56 regardless of the original format or location of the data. Semantic data integration aims at 57 combining heterogeneous data in a way that preserves the original 'meaning' of the data in 58 their particular semantic context. In practice, this often consists in establishing semantic 59 correspondences (also called *mappings*) between the vocabularies of the different data 60 sources and a common reference ontology. The result of this process is called a knowledge 61 graph.



Figure 2. The RDF data format represents factual statements about entities (here, the taxon
Entomobrya ligata) as triples that consist of a subject, predicate and object. RDF triples form
a labeled directed graph, which is why RDF databases are also called RDF graphs.

66

67 A knowledge graph (KG) is a graph-structured knowledge base that stores factual 68 information in the form of relationships between real-world entities (like people, places, 69 'things') [18]. Under the Resource Description Framework (RDF), the standard data model of 70 the Semantic Web, a KG is a set of (subject, predicate, object) triples. A RDF triple is a 71 factual statement about an entity (the subject), connected to another entity or a data value 72 (the object) by a relationship (the predicate). A set of RDF triples forms a labeled directed 73 graph, called a RDF graph (Figure 2). But not every RDF graph is a KG. The triples in a KG 74 can be separated into two distinct, yet connected, layers (Figure 3). The schema layer is the 75 conceptual model of the KG and is described by an ontology or a collection of ontologies. An 76 ontology is a formal shared conceptualization of a domain of interest [19]. It defines a 77 common agreed upon terminology in terms of concepts (also called *classes*, i.e. the types of 78 things that exist in the domain) and the relationships holding among them. An ontology is 79 specified using a logic-based ontology language — most often the Web Ontology Language 80 (OWL), built upon RDF — that allows both humans and computers to understand the 81 semantics ('meaning') of the data. The data layer holds the concrete, factual data. These 82 data are *instances* of the general concepts (classes) defined in the ontology. For example, if 83 we were to define a class 'Article author' in a hypothetical ontology to describe the concept

of 'people who write scientific papers', then 'Nicolas Le Guillarme' and 'Wilfried Thuiller' would be two instances of this class. In the context of semantic data integration, the data layer of a KG is populated with instance data from multiple sources. The ontology is used to link these disparate datasets at the schema-level, acting as a mediator for reconciling the structural and semantic heterogeneities between data sources.





90

91 Figure 3. A knowledge graph is a graph database that embeds both the data and its 92 semantics in two interconnected layers. The schema layer is an ontology or a collection of 93 ontologies that integrate datasets at the schema-level and allow logical inference of implicit 94 knowledge using specialized softwares called reasoners. The data layer is a collection of 95 data from various sources.

96

97 KGs have a number of advantages over other types of databases, such as relational ones. 98 Their graph structure allows for efficient querying, intuitive visualization, and analysis using 99 graph algorithms or relational machine learning [18]. Using an ontology as a schema layer, 100 KGs embed a formal semantics with the data which can be used by computers to interpret 101 and reason about the data, thus potentially allowing to infer new facts (e.g. the inferrable 102 relationships in Figure 2). KGs make it easy to integrate new types of data by altering the 103 ontology or adding a new ontology to the schema layer. When following the Linked Open Data principles [20], domain-specific KGs can be easily interconnected into larger (possiblycross-domain) KGs.

106 KGs have recently become prevalent as a framework for semantic data integration in many 107 different domains of science and industry [21]. It was R. Page, in his seminal 2016 paper, 108 who first suggested the use of KGs in the biodiversity field [22]. Since then, only a few 109 examples of biodiversity KGs have been published. Ozymandias [23] is a KG for the 110 Australian fauna that integrates data from several sources, including the Atlas of Living 111 Australia, the Australian Faunal Directory, the Biodiversity Heritage Library and the 112 Biodiversity Literature Repository. OpenBiodiv [24] integrates information extracted from the 113 biodiversity literature into a graph database using the OpenBiodiv-O ontology and an RDF 114 version of the Global Biodiversity Information Facility (GBIF) taxonomic backbone. TAXREF-115 LD [25] is a KG representation of the French national taxonomical register for fauna, flora 116 and fungus that interlinks information about taxonomy, species interactions, development 117 stages, biogeography, conservation statuses, etc. In a recent talk at TDWG 2021, Michel et 118 al. [26] called for more biodiversity data producers to start publishing KGs. However, for 119 now, building a KG from multiple data sources is a complex and time-consuming task that 120 demands high Semantic Web expertise, and we are not aware of an existing tool specifically 121 designed to help ecologists transform their data sets into interoperable KGs - with the 122 notable exception of the iKNOW project [27], which is very similar in spirit to our work, but 123 whose current status is unknown to us.

124 In this paper, we present inteGraph, a framework and toolbox that facilitates the process of 125 building a KG from heterogeneous and distributed (semi-)structured data sources in the 126 biodiversity domain. With inteGraph, users can create automatic and reproducible semantic 127 data integration pipelines simply through the provision of configuration files. This declarative 128 approach requires no (or little) code from the user and minimizes the amount of manual 129 effort and Semantic Web expertise required to turn datasets into interoperable KGs.

130 To illustrate our approach, we will show how inteGraph can be used to integrate data on the 131 trophic ecology of soil organisms from multiple sources into a KG that can support 132 multitrophic studies. Multitrophic studies, spanning multiple trophic levels and/or taxonomic 133 groups, are essential to identify general patterns in community ecology [28], understand how 134 diversity is related to ecosystem stability and ecosystem functioning [29], and provide the 135 necessary guidance with biodiversity loss and environmental problems [30]. Multitrophic 136 approaches should acknowledge the complexity of ecosystems while remaining practical. 137 Large trait databases have the potential to address this trade-off between feasibility and 138 completeness. By supporting the assignment of species (or higher taxonomic ranks) to 139 trophic and/or functional groups, they reduce the dimensionality of ecological communities 140 without biasing studies toward a single trophic level or taxonomic group [31, 15]. Yet, some 141 challenges still remain. Although we have trait databases available for some groups of soil 142 organisms, our trait knowledge is limited for most of them. In addition, existing databases 143 tend to function as data silos whose lack of interoperability can discourage researchers to 144 include more trophic levels and/or taxonomic groups in their studies.

145 The ability to create a KG integrating trophic information from a number of trait databases 146 covering different soil taxonomic groups across several trophic levels could greatly facilitate 147 multitrophic studies in soil ecology research. Such a trophic KG would provide a unified 148 access to multigroup, multitrophic, and multisource information. The integration of several 149 trophic datasets (e.g. a first one containing information on carabid diets and a second one 150 focusing on the feeding habits of springtails) into a KG allows the use of a single query to 151 retrieve all organisms with a particular diet, regardless of the format, location or taxonomic coverage of the original data source. KGs also offer the ability to reason about the integrated 152 153 data to derive additional knowledge. Reasoning about trophic interactions and dietary data opens the way for automatic classification of soil organisms into trophic groups, which can 154 155 facilitate the reconstruction of consistent soil food webs from multisource data. This will be 156 illustrated with examples in the Results section.

157 Material and Methods

158 Overview of the approach

Figure 4 is a high-level representation of our approach to constructing a KG from heterogeneous and distributed (semi-)structured data sources. At the heart of our framework is inteGraph¹, an open-source toolkit for ontology-based data integration in the biodiversity domain that allows generating data integration pipelines dynamically from configuration files and scheduling and monitoring the execution of these pipelines.





166 Figure 4. A high-level representation of the proposed declarative approach for constructing a

- 167 knowledge graph from distributed (semi-)structured data sources.
- 168 Data sources

Data sources can be (and often are) distributed on several machines, on a local network and/or on the web. Data must be accessible in a (semi-)structured form, for instance as tabular (e.g. tables in relational databases or in CSV files) or hierarchical data (e.g. data in XML or JSON format). At present, inteGraph does not include information extraction components that would allow the integration of unstructured textual data from the literature.

9 1 Available at https://github.com/nleguillarme/inteGraph

174 In our running example, we will use inteGraph to build a trophic KG from the following three175 data sources:

The Fun^{Fun} database [13] collates fungal functional trait data, including information about trophic guilds, from a variety of sources, for thousands of species across the fungal tree of life. Data are provided in a tabular format (CSV file) and can be downloaded from Zenodo (<u>https://zenodo.org/record/1216257</u>).

- BETSI [11] is an open database gathering data on morphological traits and ecological preferences for 7 taxonomic groups of soil invertebrates (Aranae, Carabidae, Chilopoda, Collembola, Diplopoda, Isopoda and Diplotesticulata) from about 2000 literature references. BETSI is accessible on demand via a web portal (https://portail.betsi.cnrs.fr) that provides the user with an interface to write queries and download subsets of the database in a tabular format (CSV file). In the following, we will integrate a dataset containing Carabidae diet data.
- 187 The Global Biotic Interactions (GloBI) provides open access to species interaction 188 data (e.g. predator-prey, pollinator-plant, pathogen-host, parasite-host) aggregated 189 from existing open datasets [32]. As of April 2023, GloBI contains over 17M 190 interaction records obtained from 342 datasets, covering 823,033 taxa. GloBI 191 provides several ways to access its data, including а web portal 192 (https://www.globalbioticinteractions.org/), a downloadable snapshot of the entire 193 database in a tabular format (CSV file), and a web API. In our example, we will use the web API to download data about the trophic interactions of Collembola. 194

195 Information from these three data sources will populate the data layer of our trophic KG once196 it has been transformed into a common representation.

197 Target ontology

198 InteGraph adopts a top-down approach to KG creation. In this type of approach, the schema 199 layer of the KGis populated with a predefined ontology. The semantic data integration 200 process then consists of populating the data layer of the KG with data extracted from the different data sources, and creating semantic links between the schema of the sources andthe (global) schema of the KG using mapping rules.

203 To reconcile schematic and semantic heterogeneities between our trophic data sources, the 204 schema layer of our example KG will be populated with two ontologies: the NCBITaxon 205 ontology and the Soil Food Web Ontology (SFWO) [7]. NCBITaxon is a formal translation of 206 the NCBI Taxonomy database into an ontology, in which each taxon is treated as a class 207 whose instances would be individual organisms, e.g. 'Nicolas Le Guillarme' instance of 208 NCBITaxon_9606 (Homo sapiens). To our knowledge, the NCBI Taxonomy database is the 209 only taxonomic nomenclature available as an OWL ontology. SFWO is an ontology for 210 representing knowledge on the trophic ecology of soil organisms across taxonomic groups 211 and trophic levels. SFWO captures the semantics of trophic concepts such as trophic 212 interactions, feeding processes, diets or trophic groups. SFWO also includes machine-213 interpretable definitions for most of these concepts, that allow for inference of implicit 214 knowledge using automated reasoning, e.g. deducing a consumer's diet(s) from the trophic 215 interaction(s) in which it participates.

216 Triplestore

A triplestore is a database management system, i.e., a software used for storing and querying a database, specifically designed to support the storage and the efficient querying of RDF triples. A triplestore is needed to store both the schema and data layers of a KG. Information stored in the triplestore can be retrieved using SPARQL queries. A multitude of triplestore implementations are available (see [33] for a survey), which offer different capabilities and performance in terms of data storage and indexing, query processing, reasoning, etc.

InteGraph assumes the existence of a running triplestore instance. It is not tied to a specific implementation and provides connectors to several triplestore solutions. The user is expected to provide connection information as part of the pipeline configurations. As a top227 down approach, inteGraph assumes that the target ontology has been loaded in the 228 triplestore before the data integration process starts.

To store our example knowledge graph, we will use GraphDB Free², a RDF triplestore solution that can manage billions of explicit statements on a desktop hardware, while providing optimized query evaluation and OWL reasoning.

232 Configuration files

InteGraph implements a declarative approach to building KGs, which means that it provides control over the creation and execution of semantic data integration pipelines using configuration files. InteGraph requires the user to provide two types of configuration files: a single graph configuration file (Figure 5a), and a set of source configuration files, one for each data source (Figure 5b).

The graph configuration file contains global information, including the name of the KG (that acts as a prefix to create an identifier for each graph generated from a data source), the name of the directory containing the source configuration files, the triplestore connection information, and the declaration of the target ontologies.

The source configuration file is where the user specifies the information needed by inteGraph to instantiate the Extract and Transform components of the data integration pipeline for a given source. This includes:

- the internal identifier of the data source;
- data access information, which determines the type of data source file-like or HTTP
 and the appropriate data extraction component to be added to the pipeline;
- information about the format of the input data, e.g. tab or comma-separated values;
- the path to an (optional) data cleansing script;

for each entity (e.g. taxon, trait) in the input data, the name of the columns containing
 information about the entity (label and/or identifier), and a sequence of semantic

14

annotation components whose role is to map the entity to its equivalent in the target

253 ontology;

254

• the path to the spreadsheet containing the schema mapping rules.

[core]	[core]
base_iri=http://leca.osug.fr/example	source_id=funfun
[sources]	[extract]
dir=sources	[extract.file]
	file_path=https://github.com/traitecoevo/fungaltraits/
[load]	releases/latest/download/funtothefun.csv
id=graphdb	
conn_type=http	[transform]
host=0.0.0.0	format=csv
port=7200	delimiter='",'
user=integraph	chunksize=1000
password=iNtEgR@pH	
repository=example	[transform.cleanse]
	script="clean.py"
[ontologies]	
sfwo=https://purl.org/sfwo/sfwo.owl	[transform.annotate]
	[transform.annotate.taxon]
	label=speciesMatched
	id=ifungorum_number
	source=ifungorum
	target=[''ncbi'']
	[transform.annotate.guild]
	label=guild_fg
	target=[''stwo'', ''mapping.yml'']
	[transform.triplify]
	mapping=mapping.xlsx

(a) Graph configuration

(b) Source configuration for the Fun^{Fun} database

255 Figure 5. InteGraph implements a declarative approach to KG construction, giving the user

256 control over the creation of data integration pipelines through simple configuration files.

257



Figure 6. An illustration of the application of data transformation to our example datasets (D1: Fun^{Fun}, D2: Carabidae diet data from BETSI, D3: Collembola trophic interaction data from GloBI). Figure 6d shows the set of RDF triples (in N-quads format) generated from the first row of each data table.

263 Anatomy of inteGraph pipelines

264 InteGraph pipelines are structured according to the Extract-Transform-Load (ETL) paradigm. 265 An ETL pipeline collects data from an input source (extract), cleans and maps the data from 266 a source schema — the schema of the original data source — to a target schema 267 (transform), and saves the transformed data into a triplestore (load). In a typical ETL 268 process, a copy of the extracted data is stored in a data staging area and all transformations 269 are applied to the staged data. In inteGraph, an ETL pipeline is dynamically created at 270 runtime for each data source from the configuration files provided by the user. This ETL 271 pipeline extracts and stages the raw data from the data source, transforms the staged data 272 into a RDF graph, and loads the RDF graph into the data layer of the triplestore.

273 Data extraction

This first step of the ETL data integration process involves collecting data from the data source. InteGraph implements a number of components to connect to different types of data sources. At the moment, inteGraph supports the following types of data sources:

File-like data sources: inteGraph can download files from remote or local file-like
 sources by specifying the local path or the URL of the source in the configuration.
 Archive files, including compressed archives, are supported, and unpacked before
 staging.

HTTP data sources: inteGraph can extract data from remote databases exposed
 through a web-based API by sending HTTP GET requests to the API endpoint. In
 that case, the user is expected to provide the URL of the endpoint and the query
 string. Paginated results are supported using the limit and offset parameters.

These two components alone are sufficient to access most ecological datasets. We plan to add more connectors in the future, including connectors to SQL databases, RDF databases, etc. The extracted data are staged on the local file system.

Figure 6a shows the data extracted from our three example data sources. The three datasets use different data structures and terminologies to organize and describe taxonomic and trophic information.

- The Fun^{Fun} database uses the Index Fungorum taxonomic nomenclature. Each line of
 the data table contains a single trait information for a given taxon. The name of the
 trait is given in the trait_name column and its value(s) is given in the value column.
 The terminology used to describe the guild of each taxon is inherited from the
 FunGuild database.
- BETSI does not encode taxonomic information using identifiers from a reference taxonomy. Taxa are designated only by their scientific name. Similar to Fun^{Fun}, each line of the data table contains a single trait information for a given taxon. The diet terminology is taken from the T-SITA thesaurus [4].

Each line in GloBI's data table contains information about a single interaction. The interaction is directed, so each line contains information about the source and target taxa (names and identifiers in an external reference taxonomy, e.g. ITIS, NCBI, GBIF...) and the interaction name. GloBi maintains a mapping between different taxonomic nomenclature internally, but each taxon in the data table is linked to a single identifier. The target of the trophic interaction can also be a non-taxonomic onteraction.

307 Data transformation

The second step of the ETL data integration process involves transforming the staged data into a RDF graph, i.e. a set of RDF triples. In inteGraph, data transformation consists of two successive operations: data cleansing and schema mapping. 311 Under the term data cleansing, we include all the dataset-specific data processing 312 operations that aim at formatting the extracted data so that they are ready for further 313 processing by the schema mapping component. This includes operations such as removing 314 or filling missing values, removing duplicates, dropping irrelevant data, splitting strings (i.e. 315 splitting a string representing a set of values, e.g. 'bacterivore-detritivore', into a set of 316 strings, each string representing a single value, e.g. 'bacterivore', 'detritivore'), joining two or 317 more data tables, etc. Figure 6b shows an example of applying cleansing operations to the 318 Fun^{Fun} dataset so that each line of the data table contains a single guild value. As possible 319 cleansing operations are very diverse and highly dependent on the structure of the input 320 data, they cannot be specified in the source configuration file. Instead, the user should 321 provide a Python or R script that implements the data cleansing operations as a separate 322 file. This script should respect some input/output constraints so that it can be ingested by 323 inteGraph at runtime and incorporated into the ETL pipeline.

324 After data cleansing is complete and cleansed data are staged, the pipeline moves on to 325 schema mapping which involves converting data from the schema of the original data source 326 to the schema of the knowledge graph, i.e. the target ontology. Schema mapping in 327 inteGraph consists of two successive tasks: semantic annotation and RDF graph generation. 328 Semantic annotation is the process of linking the input data with the concepts in the target ontology that best capture the semantics of the data (Figure 6c). InteGraph provides several 329 330 components for semantic annotation of biodiversity data. The first component maps 331 taxonomic entities (identified by their name and/or identifier in a source taxonomic nomenclature) to a target taxonomy — in our running example, the NCBITaxon ontology. 332 333 Taxonomic mapping uses GNparser [34] to parse scientific names and nomer [35] to match 334 taxon names and identifiers to their equivalent in the target taxonomy. The second 335 annotation component allows any entity (e.g. trait name, trait value, interaction type) to be 336 linked to concepts in a target ontology using exact string matching. For instance, to link the term 'Plant pathogen' found in the Fun^{Fun} database to the corresponding class in the Soil 337 338 Food Web Ontology, the component will retrieve all the classes whose label (or the label of one of its synonyms) matches exactly the lookup term. If a single eligible class is found, the term in the input data is annotated with this concept identifier, here SFWO:0000159 which is the identifier of the class 'plant pathogen' in SFWO. A third annotation component allows the user to provide a YAML file containing a dictionary with term:concept pairs. Semantic annotation components can be chained together to handle mismatched terms (see the source configuration file example in Figure 5b). Figure 6c shows the result of applying semantic annotation on our example datasets.

346 Once the relevant data have been linked to the corresponding concepts in the target 347 ontology, the final step of schema mapping is the conversion of the annotated dataset into 348 an RDF graph (Figure 6d). InteGraph uses RDF Mapping Language (RML) [36] rules to 349 transform tabular data into RDF triples. RML is a declarative language for expressing rules 350 that map data in heterogeneous structures to the RDF data model. These rules describe the 351 desired graph structure, that is how the data and schema layers of the graph should be connected to each other. The schema mapping rules should be provided by the user as part 352 353 of the data source configuration. However, writing RML mapping documents is beyond the reach of most non-expert users. To face this issue, inteGraph enables to specify mapping 354 355 rules in spreadsheets that are automatically translated into RML documents using 356 Mapeathor [37] (Figure 7). This provides a more user-friendly manner to declare mapping 357 rules in a language-independent way. Finally, inteGraph applies Morph-KGC [38], a modern 358 RML processing engine with a focus on speed and scalability, to execute the RML mapping rules and generate the RDF graph. Morph-KGC uses the RML rules to determine how the 359 annotated data should be transformed into RDF triples. The RML rules are applied to each 360 361 row in the annotated data to generate the RDF representation of the information in the row. 362 In case of missing data (e.g. a taxonomic entity that could not be mapped to the target 363 taxonomic), the RDF triples that use the missing data are not materialized. RML rules 364 processing results in a RDF graph which is the sum of the sets of RDF triples generated for 365 each row. Figure 4d shows an extract of the RDF graphs obtained by applying RML rules to 366 our example datasets. RDF graphs are staged in N-quads format, a serialization format for 367 RDF data that associates each triple with an optional context value at the fourth position.
368 This context value takes the form of a graph label, indicating which RDF graph the triple
369 belongs to. This graph label is used to keep track of the data provenance (original data
370 source) after the different RDF graphs are merged into a single KG in the triplestore.

371



373 Figure 7. InteGraph allows the user to specify schema mapping rules in a spreadsheet, 374 which are automatically converted into RML rules using Mapeathor. The RML rules are 375 executed using Morph-KGC to generate the RDF graph.

376 Data loading

377 The third and final step of the ETL data integration process is to save the RDF graph 378 generated during the data transformation stage in an external RDF database, i.e. a 379 triplestore. The triplestore must be set up beforehand, either on the same machine running 380 inteGraph or on a dedicated server. Different triplestore implementations may use different 381 techniques to ingest RDF data. InteGraph provides connectors to the following triplestore 382 solutions: RDFox, GraphDB, and Virtuoso. InteGraph also supports loading RDF data to a 383 triplestore using SPARQL Update operations. In our example, the trophic KG is stored on an 384 instance of GraphDB Free. The GraphDB connector provided by inteGraph simply loads RDF data to the triplestore using an HTTP POST request. 385

386 At the moment, inteGraph supports full load only. This means that the transformed data are 387 loaded in full at each run of the ETL pipeline. Therefore, the KG is reconstructed from scratch every time the data integration pipelines are executed. A useful alternative would be incremental data load, i.e. updating the KG at regular intervals by loading only the data that has changed (new or updated data) since the last execution. This requires additional tools to compare the data from the data source with the existing data present in the KG. Incremental data load has a number of advantages over full load, including faster processing and preservation of data history.

394 Pipeline creation, scheduling and monitoring

InteGraph uses Apache Airflow³ to schedule and monitor the execution of the data 395 396 integration pipelines. Airflow provides a flexible programmatic (i.e. code-based) approach to 397 easily build scheduled data processing pipelines as directed acyclic graphs (DAGs) of tasks. 398 DAGs are a natural representation for ETL pipelines as each step in the ETL process is 399 executed after the previous one has been completed (there is no circular dependency 400 between ETL tasks). Tasks in Airflow should be atomic – they either succeed and produce 401 some proper result or fail in a manner that does not affect the state of the system - and 402 idempotent, i.e. rerunning a task without changing the inputs should not change the overall 403 output.

404 At runtime, inteGraph parses the graph and source configuration files and creates one 405 Airflow pipeline per data source, decomposing the full ETL pipeline into a DAG of atomic and 406 idempotent tasks. A schedule interval can be assigned to each pipeline, which determines 407 when and how often the pipeline is run. Alternatively, the user can manually trigger the 408 execution of a pipeline in Airflow's graphical user interface. This interface also allows to 409 visualize the pipelines generated by inteGraph and monitor their execution (Figure 8). Airflow 410 can handle failures in ETL operations by retrying them a couple of times. If the error persists, 411 the user can easily explore the logs of the failing task, identify the cause of the failure, and 412 rerun the failing task (together with any subsequent tasks that depend on that task). Airflow 413 also has the ability to run multiple tasks in parallel. Therefore, pipelines can be executed 22 3 https://airflow.apache.org/

efficiently, taking advantage of any parallelism inherent in the tasks dependency structure.
For example, inteGraph can split the input data into chunks that are transformed in parallel
and merged before loading, reducing pipeline execution time. In addition, ETL pipelines can
run in parallel as each data source is independent of the others.

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Airflow DAGs Datasets Security Browse Admin Docs		14:43 UTC - AA -
DAG: funfun	None Schedule: @once	Next Run: 2023-04-19, 00:00:00
🖽 Grid 📑 Graph 🖬 Calendar 📲 Task Duration 🛱 Task Tries 🖄 Landing Times 📃 Gantt 🛕 Details	<> Code 🚯 Audit Log	
Image: Second state	ns yet.	Find Task
BashOperator BranchPythonDecoratedOperator PythonDecoratedOperator deferred failed queued removed restarting running scheduled shutdown	skipped success up_for_reschedule	up_for_retry upstream_failed no_status
		Auto-refresh C
extract → cleanse → annotate → generate_graph →	load	

420 Figure 8. A high-level view of the ETL pipeline for the Fun^{Fun} database in the Airflow user 421 interface.

422 Results

423 Knowledge retrieval

424 At the end of the semantic data integration process, the target ontology and the transformed 425 data are both saved in a single triplestore. The triplestore is responsible for storing the KG 426 and executing SPARQL queries to retrieve information from it. SPARQL is a query language 427 for retrieving and manipulating data stored in RDF format. SPARQL is based on matching 428 graph patterns against the RDF graph. The basic graph pattern is the triple pattern, which is 429 like a RDF triple where any part of the triple can be replaced by a variable. A graph pattern is 430 a combination of such triple patterns. When executing a SPARQL query against a KG in a 431 triplestore, the triplestore searches for the set(s) of triples that exactly match the graph 432 patterns defined in the query, regardless of the provenance (i.e. the original source) of the 433 triples, unless explicitly requested. This means that the set of RDF triples returned in 434 response to a SPARQL query may contain facts originating from different data sources. The 435 KG provides the user with a unified view of the original data sources through querying, and 436 enables combining multisource information as part of a query response. Figure 9 shows a 437 SPARQL query searching the KG for phytophagous species. The same query returns both 438 springtail and carabid species, whose dietary information originates from the GloBi and 439 BETSI databases respectively. This simple example shows how a single query against the 440 KG can retrieve information from multiple sources simultaneously, thus greatly facilitating 441 integrative studies across taxonomic groups and/or trophic levels.

442

443



Sminthurinus aureus	
Sminthurus viridis	
Sphaeridia pumilis	1
Sminthurinus niger	
Dicyrtoma fusca	
Bourletiella hortensis	
Orchesella villosa	
Pseudoophonus griseus	XX
Harpalus griseus	E B
Amara eurynota	7 (

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445 Figure 9. Example of a SPARQL query returning the species names of phytophagous taxa. ?

446 x denotes a variable called x. The LIMIT keyword is used to limit the number of results to the

first 10 entries. The query returns information about both phytophagous springtails (from the
GloBi database) and phytophagous carabid beetles (from the BETSI database).

449 Making implicit knowledge explicit

450 The semantic data integration process builds a KG by linking heterogeneous datasets at the 451 schema level using an ontology. During the process, the data layer of the KG is populated 452 with the factual information stated in the different datasets and transformed into knowledge 453 through semantic annotation and transformation into a RDF graph. Based on these explicit 454 facts, additional knowledge that is not explicitly present in the data can be derived using 455 reasoning. This ability is a direct consequence of OWL (the standard language for specifying 456 ontologies) being based on a subset of first-order logic. Therefore, automated reasoners can 457 be employed to evaluate the logical implications of the knowledge encoded in the ontology 458 on the explicitly stated data.

459 There are two principle strategies for logical inference: forward chaining and backward 460 chaining [38]. Forward chaining, also known as materialization, derives all the facts that can 461 be logically deduced from the existing facts and a set of logical rules, and stores these 462 inferred facts in the triplestore for later querying. Precomputing all inferred facts enables 463 efficient query answering, but it can also be very expensive both in time (the materialization 464 process needs to consider all possible inferences) and memory (the process can derive a 465 large number of facts). In addition, materialization must be redone each time the data is 466 updated.

Backward chaining (query rewriting) starts from a query and applies the logical rules only as far as they are needed to answer the query. With backward chaining, reasoning is done at runtime and no time- and space-consuming precomputation is needed. Furthermore, no recomputation has to be done when the data is updated. However, a major drawback of backward chaining is that reasoning must be done for each new query, which can be computationally expensive and slow. 473 In our running example, the target ontologies (the NCBITaxon ontology and the Soil Food 474 Web Ontology) are loaded in a triplestore supporting reasoning based on forward chaining. 475 The Soil Food Web Ontology provides a set of logical rules that map consumer-resource 476 interactions to diets (e.g. an animal feeding on detritus is a detritivore), as well as rules for 477 classifying soil-associated consumers into hybrid taxonomic-trophic groups (e.g. 478 detritivorous springtails are members of the group Collembola.detritivores). These rules 479 make it possible to automate the process of assigning taxa to trophic groups using logical 480 inference, thus reducing the burden of manual trophic group assignment.

481 Figure 10 illustrates how information about trophic group membership is made explicit in our 482 trophic KG using materialization. After transformed data are loaded in the triplestore at the 483 end of the data integration pipeline, inference rules are applied repeatedly to the asserted 484 (explicit) statements until no further inferred (implicit) statements are produced. Given (1) the 485 explicit information about Entomobrya ligata feeding on rotting wood (see first line of data table D3 in Figure 6a), (2) the hierarchy of taxonomic concepts provided by the NCBITaxon 486 ontology, and (3) the logical rules provided by the Soil Food Web Ontology, the triplestore 487 488 reasoner is able to materialize the following logical implications:

- 489 *E. ligata* is a species of springtails (Collembola);
- 490 E. ligata is a detritivore, as it feeds on rotten wood, which is a type of detritus ;
- *E. ligata* belongs to the group of detritivorous springtails (Collembola.detritivores) as
 a logical consequence of the two previous assertions.
- 493



tg_iri	tg_name
http://purl.org/sfwo/SFWO_0000302	Collembola.all
http://purl.org/sfwo/SFWO_0000304	Collembola.detritivores

496 Figure 10. Example of a SPARQL query returning the trophic groups to which Entomobrya 497 ligata belongs. A trophic group is defined in the Soil Food Web Ontology as 'a collection of 498 organisms that feed on the same food sources and have the same consumers' [7, 31]. 499 SFWO provides a logical formalization of the hierarchical classification of soil consumers 500 proposed in [39].

501 Performance

502 InteGraph relies on a number of external tools with a strong focus on scalability (e.g. 503 GNparser for scientific name parsing, Morph-KGC for RML rules execution). This, combined 504 with Airflow's ability to run independent tasks in parallel, makes inteGraph itself quite 505 efficient at handling large datasets in a reasonable time. In our experiments, we were able to 506 convert tabular data with over 440K rows into an RDF graph in about 6 minutes on a laptop 507 with twelve 2.60GHz Intel Core i7 CPUs and 16GB of RAM. Currently, the main bottlenecks 508 are taxonomic mapping, which in some cases may require many calls to web APIs, and 509 logical inference, the performance of which depends on the types of reasoning and the 510 optimisations implemented by the triplestore (inteGraph provides no reasoning component, 511 the inference is left entirely to the triplestore).

512 With the ability to chain semantic annotation components, including user-provided dictionary-513 like mapping files, inteGraph is able to convert most of the input data into RDF, with however 514 some entries being dropped because they cannot be linked to concepts in the target 515 ontology. Most of the time, this happens because the taxonomic entities could not be mapped to the target taxonomy. This can be due to the source and target taxonomies being 516 incompatible, the taxon name being ambiguous or deprecated, etc. For example, in the 517 518 FunFun database, 41 of the 508 unique taxa could not be mapped to the NCBITaxon 519 ontology, resulting in 15% of the input data being dropped during the data integration

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520 process. In the Carabidae dataset extracted from BETSI, this proportion is only 0.3% (with 521 18 of the 5491 unique taxa for which inteGraph could not find a correspondence in the 522 NCBITaxon ontology).

523 Discussion

524 Multitrophic studies require harmonizing and integrating datasets across a large variety of 525 taxonomic groups and trophic levels. Despite considerable efforts to make more biodiversity 526 data freely available in a (semi-)structured format, the multiple dimensions of data heterogeneity (semantic, structural, syntactic) constitute a major obstacle to the 527 528 interoperability of data sources [3]. Here, we introduced a practical approach to data 529 integration that aims at making heterogeneous and distributed biodiversity data sources 530 interoperable as part of a single KG. KGs provide a unified representation of disparate data 531 sources and allow for retrieving data across these sources using a single guery. By using 532 ontologies as global schemas, they add semantics to the integrated data, making it easier for 533 humans and computers to interpret the data and for reasoners to infer additional facts. As 534 seen from the example discussed in the Results section, the ability to reason about the data 535 in our trophic KG opens avenues for automatic classification of soil organisms, which can 536 facilitate the reconstruction of consistent soil food webs from multisource data. In addition, 537 KGs provide support for a number of applications [41], including both in-KG, e.g. link 538 prediction, error detection, and out-of-KG applications, e.g. relation extraction from text, 539 recommender systems, etc.

540 Despite their many advantages, KG construction is currently out-of-reach for most 541 biodiversity data providers and consumers as they require in-depth expertise in Semantic 542 Web technologies. InteGraph is an attempt to make semantic data integration and KG 543 construction more accessible to the biodiversity science community. Requiring little or no 544 code and minimal knowledge of the Semantic Web, inteGraph facilitates the processes of 545 converting a biodiversity dataset into a KG and of integrating multiple datasets into a single 546 KG. Given a set of distributed data sources and a target ontology, inteGraph allows the user 547 to control the creation and execution of reproducible ontology-based data integration 548 pipelines through a set of simple configuration files. This declarative approach relieves the 549 user of the implementation burden. Instead, the user can focus on the desired structure of 550 the target KG and on the schema mapping rules needed to transform the input data into 551 RDF graphs. InteGraph relies on high-performance third-party tools (gnparser, nomer, 552 Morph-KGC, Airflow), which guarantees a certain ability to scale to large datasets. The 553 viability of our approach has been tested by creating a KG of soil trophic ecology from 554 multiple open trait databases, using the Soil Food Web Ontology and the NCBITaxon 555 ontology as the KG schema. Currently, inteGraph is at the proof-of-concept stage. It still 556 needs some development to make it more robust, scalable and user-friendly. We also plan 557 to add more advanced features in the future, especially regarding data provenance tracking 558 and continuous KG updating.

559 Although it represents a significant advance in the field of ontology-based biodiversity data 560 integration, inteGraph suffers limitations related to current practices in biodiversity data 561 management. First, inteGraph requires the data sources to provide data in a 562 (semi-)structured format through a programmatic interface, e.g. a URL to download the data 563 file or a web API that handles HTTP requests. Still lots of data about soil biodiversity are not 564 accessible this way, e.g. data from the BETSI database must be downloaded manually. We are confident that this situation will become less frequent in the future. Second, as a top-565 down approach to KG creation, inteGraph requires a predefined ontology to act as the 566 mediating schema to link heterogeneous data sources. Creating an ontology to model 567 568 knowledge in a domain of interest is a complex process that requires a significant investment 569 of time and effort. Ontology engineering asks for a group of experts to produce a consensual 570 conceptualization of the domain. For instance, in the domain of soil trophic ecology, this 571 means trying to harmonize the use of diet terms that may have different meanings from one 572 taxonomic group to another. However, we believe that the result is worth the effort, as a

573 properly designed ontology can benefit the whole community by facilitating knowledge 574 sharing, dataset standardization and, ultimately, data integration.

575 Finally, although it aims to make semantic data integration more accessible to a non-expert 576 audience, inteGraph still requires a minimum of knowledge of Semantic Web technologies 577 (RDF data, ontologies, SPARQL queries...). Just as the environmental community has 578 begun to embrace new artificial intelligence tools from recent developments in deep machine 579 learning, we encourage the community to take an interest in Semantic Web tools for better 580 biodiversity knowledge management.

581 Continuing our efforts to develop more and more biodiversity ontologies [42, 25, 43, 7] would 582 allow us to envision increasing semantification of the ecology domain in the near future. 583 Combined with tools such as inteGraph, which facilitate the conversion of biodiversity 584 datasets into graph knowledge bases, these semantic resources could support the creation 585 by different communities of numerous domain-specific KGs, which could eventually be 586 interconnected to form a single biodiversity KG covering the entire tree of life and the full 587 diversity of global ecosystems.

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Box 1. Glossary

Class: in an ontology, a description of a concept in the domain of interest.

A class is a set of individuals that share common characteristics, and the class definition gives the properties that these individuals must fulfill to be members of the class.

For instance, 'bacterivore' is the class of all individual organisms that feed on bacteria.

Extract-Transform-Load: a three-phase data integration process that combines data from multiple sources into a single central repository.

Instance (individual): a real-world realization of a concept defined in an ontology. In ontological terms, an individual is an instance of a class in the ontology.

Knowledge graph: a knowledge base that uses a graph-structured data model to integrate data.

N-quads: a line-based, plain text format for storing and transmitting RDF data. A N-quads statement is a RDF triple extended with an optional context value that takes the form of a graph label, indicating which graph the triple belongs to.

Ontology: the formal and consensual description of a domain of interest as a set of interrelated concepts.

Reasoner: a computer program that uses an ontology to infer logical consequences from a set of asserted facts.

Resource Description Framework (RDF): the standard data model of the Semantic Web. RDF represents any piece of information as subject-predicate-object triples.

RDF Mapping Language: a language for expressing mapping rules from heterogeneous data structures to the RDF data model.

Semantic data integration: the process of combining data from different sources into a single, unified view using ontologies.

Semantic Web: a set of standard technologies - including the Resource Description Framework (RDF), Web Ontology Language (OWL), and SPARQL - that help make computers better able to interpret data and information published on the web.

SPARQL: the standard query language for retrieving and manipulating data stored in RDF format.

Triplestore: a database engine optimized for the storage and retrieval of RDF data.

Web API: an interface consisting of one or more endpoints publicly exposed on the web, that allow a user to programmatically access some specific features or the data of an application, e.g. a database.

Web Ontology Language (OWL): a family of knowledge representation languages and the World Wide Web Consortium's (W3C) standard for authoring ontologies, built on RDF and characterized by formal semantics based on description logics (decidable fragments of first-order logic).

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