Support for Taxonomic Data in Systematics

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Abstract

The Systematics community works to increase our understanding of biological diversity through identifying and classifying organisms and using phylogenies to understand the relationships between those organisms. It has made great progress in the building of phylogenies and in the development of algorithms. However, it has insufficient provision for the preservation of research outcomes and making those widely accessible and queriable, and this is where database technologies can help.

This thesis makes a contribution in the area of database usability, by addressing the query needs present in the community, as supported by the analysis of query logs. It formulates clearly the user requirements in the area of phylogeny and classification queries. It then reports on the use of warehousing techniques in the integration of data from many sources, to satisfy those requirements. It shows how to perform query expansion with synonyms and vernacular names, and how to implement hierarchical query expansion effectively. A detailed analysis of the improvements offered by those query expansion techniques is presented. This is supported by the exposition of the database techniques underlying this development, and of the user and programming interfaces (web services) which make this novel development available to both end-users and programs.

This thesis is dedicated to my family.

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Chapter 1

Introduction

This thesis makes a contribution in the area of database methods for systematics and taxonomy. It consists of 8 chapters.

The focus of this thesis is on the development of database-supported query expansion mechanisms which improve the effectiveness of queries posed on the TreeBase database by the systematics community. To this aim, this Chapter leads the reader into a high level view of the requirements underlying this work, and explains why this research was needed and timely. First, a high level overview of systematics and taxonomy is given. This is followed by background information on TreeBase and other data sources which are relevant in this context. Then it explains what queries cannot be answered by TreeBase and why this is the case. Finally, the thesis structure is presented in detail.

1.1 Background

Systematics aims to increase our understanding of biological diversity through identifying and classifying organisms and using phylogenies to understand the relationships between organisms. The field has developed very elaborate and sophisticated tools for phylogeny construction, and practitioners have been very active in building new, better and faster algorithms (DeSalle *et al.*, 2002; Scotland & Pennington, 2000). However, this has not been matched with database development for long term access and storage of the phylogenies produced from these algorithms. Much of the data used in phylogenetic analysis is acquired from databases in other fields, particularly specimen data from museum collections (Zusi *et al.*, 1982) and sequence data (Scotland

& Pennington, 2000) from databases available at NCBI (Wheeler *et al.*, 2007). The results of phylogenetic analysis, namely evolutionary trees, on the other hand are not so easily accessible. Mostly, phylogenetic trees are retrieved through literature searches. The trees are buried in the pages and supplementary material sections of the journals in which they are published. The inaccessibility compounds the practicality of use. Projects such as the tree of life (Cracraft & Donoghue, 2004) aim to build a complete phylogenetic analysis of the world's biodiversity ultimately describing the history of life on earth. The informatics requirements are vast and challenging, particularly as the data collections grow in size and complexity. Confronting the information explosion requires creative new approaches to facilitating use of that information. Finding information in such data sets becomes increasingly difficult the larger the data set and, as such, data search and discovery needs to be intuitive and precise. Data retrieval through meaningful queries is paramount to the successfully delivery of the ever more sophisticated requirements of the systematics community especially now that these large scale projects are being realised.

A phylogenetic data repository (Nakhleh *et al.*, 2003) should have a good understanding of the organisms that are represented in the phylogenetic trees and support searches using species and higher taxa names. However, currently this is not the case. TreeBASE (Morell, 1996) is the only repository for phylogenetic analyses. TreeBASE does not adequately support taxonomic data retrieval.

Taxonomic data retrieval is supported in the Genbank sequence database. Genbank contains the NCBI taxonomy and queries can be performed to retrieve data using taxon names. In contrast to NCBI, TreeBASE does not contain a taxonomy and queries selecting all *Drosophila* studies or phylogenetic trees for insects are not as easily specified. The inclusion of a taxonomic infrastructure within TreeBASE is essential in order to support these sorts of queries. This thesis aims to address the limitations of TreeBASE by providing an infrastructure to support taxonomic queries.

1.2 Taxonomy

Taxonomic data are produced by the processes of *Naming*, which involves attaching a label to a concept for the purposes of communication, and *Classification*, that is arranging similar concepts together for the purpose of organisation. The name provides a handle on the biological organism and the position in the classification provides knowledge of the organism in terms of its similarity to others (Jeffrey, 1989). This section gives a brief overview of the difficulties users experience when utilising taxonomic data.

The taxonomic classification system is an information storage and retrieval system (Mayr, 1998), originally designed to be easily memorised (Cain, 1958). Taxon names serve two roles; the name represents an organism that was described and named by a taxonomist and the name is also placed in a hierarchy to relate the organism to the tree of life. This duality presents difficulties in the use of taxonomic names. The interdependence between the name and the classification, the fact that names are not necessarily unique to one organism and also that the placement of an organism's name into the hierarchy is not fixed, all complicate the use of taxonomic names for information storage and retrieval. Compounding this is the distributed nature of the data. The Global Biodiversity Information Facility lists over 200 data sources (http://data.gbif.org/datasets/). This number will continue to grow as herbariums and museums digitise their collections (Soberón & Peterson, 2004) and make their data accessible on the web. Although taxonomy has firmly taken its place as a digital science, data accessibility continues to cause difficulty; with the distribution there is also the heterogeneity of the data and the lack of one all encompassing taxonomic reference. Given that the amount of data is growing and is in constant flux, it is unlikely that it will be possible to agree on a "unitary taxonomy" (Scoble, 2004). However, a single all encompassing data source is achievable, and this challenge is being addressed by GBIF (Saarenmaa, 1999) and projects such as the Encyclopaedia of Life (Wilson, 2003).

Most taxonomic data systems were developed to meet particular requirements in their use or data scope. In contrast to the bioinformatics sequence databases, taxonomy data is by its nature distributed. The data produced from taxonomic research tends to follow a particular focus, a group such as insects or birds, or a geographical location, and or a period in history. There is significant heterogeneity in data models and storage format of the data and the interfaces provided to access the data. The taxonomic community have recently established the Taxonomic Databases Working Group (TDWG) to address data standards, data integration and interoperability. This effort is beginning to alleviate some of the accessibility and interoperability problems experienced by users (International Union of Biological Sciences, 2006).

Taxonomic data are also not easily deployed outside the systems in which they are stored. This is due to the nature of taxonomic names. As stated by Thiele & Yeates (2002), taxa are not facts like the data in most other databases, instead, taxa are hypotheses which are "proposed, used, modified, and then perhaps discarded, as evidence dictates". The classification of an organism is based on a set of criteria selected by the expert taxonomist. Different criteria are used by different taxonomists, for example different morphological characteristics can be given different weight and trees based on molecular data can be very different to trees based on morphological data (Hedges & Sibley, 1994). Additional complications arise from the addition of new data as new organisms are discovered, and taxonomic revisions that are made to update existing groups. There can be, at any one time, more than one accepted taxonomic opinion on the name and classification of an organism. This complicates the use of taxon names as search terms. When a search is performed on the term Aves, we need to know whether the user requires the NCBI meaning of the term or the ITIS meaning of the term. Also, in situations where a name has changed for taxonomic reasons, such as *Diomedea albatrus* which was changed to *Phoebastria albatrus* (Coues, 1866), additional support is needed to recognise that these two terms are linked through synonymy. When the user performs a search on *Phoebastria albatrus*, should any data associated with *Diomedea albatrus* also be returned? Similarly, when a user performs a search on a vernacular term "short-tailed albatross", is it assumed that the system should translate this term to the appropriate Latin names, i.e. *Phoebastria albatrus* and *Diomedea albatrus*? It is not surprising that at the time of development the TreeBASE developers shelved these taxonomic issues. It is now timely and important to address the taxonomic requirements of TreeBASE, given that the system is in the process of being overhauled by the CIPRES project (CIPRES, 2006).

1.3 Systematics

Like taxonomists, most systematists focus their research on a particular group. For these scientists the taxonomic requirements are fairly manageable, and usually involve the most up-to-date checklists. Most scientists are adept at keeping up-to-date with the literature in the area and for the most part they produce their own data. Some systematics studies, however, go beyond the usual boundaries of collecting data and building trees. Two examples are cospeciation analysis (Page, 2002) and the study of species richness (Gaston, 2000).

A cospeciation study usually follows two taxonomic schemes: one for the host species, and one for the parasites. Parasites are of particular interest in systematics because of the shared history of the host and the parasite (Page, 2002). The analysis involves comparing the phylogenies of the parasite and the host. These phylogenies either need to be collected from the literature or built from morphological or sequence data. For the data that are collected, literature searches are normally conducted using the species or higher taxa names as the search terms. Similarly, a study of the parasite species richness of a group of organisms also uses two taxonomic schemes and involves collecting data using taxon names as search terms (Nunn *et al.*, 2003). This type of analysis shows that more studies now require gathering not just previously published data in order to stay up-to-date, but also for further analysis. Another example, where collecting data is integral to the study, is in building super trees (Bininda-Emonds, 2004).

Within super tree analyses, data from several studies are gathered using taxon names as search terms. Once these data are collected, the taxonomic names across these data need to be synonymised. Usually, this is done through one authoritative source, for example, Beck *et al.* (2006) used Mammal Species of the World (Wilson & Reeder, 1993); and Thomas *et al.* (2004) used the taxonomy of Monroe & Sibley (1997). Where one such data source exists, this is a simple task, however, the time is approaching when super trees go beyond the use of one taxonomic source (Cracraft & Donoghue, 2004).

The main use of taxonomic data outside its immediate user community is in information retrieval as the examples above show. Names are used as the keys to retrieve data (Garrity & Lyons, 2003; Knapp, 2000; Petsko, 2002). Currently, no one taxonomic data provider supports the needs of the systematics community. This following section describes the taxonomic requirements of TreeBASE, and provides details of the motivation for this PhD research.

1.4 TreeBASE

TreeBASE (Morell, 1996) is a phylogenetic and evolutionary information store, containing phylogenies for more than 56,000 taxa. Submission to TreeBASE is mainly voluntary but some journals require or recommend that authors submit data to TreeBASE. TreeBASE is unique in that it stores all the data that are required to reproduce the analysis, including aligned data sets, the weighting schemes and step matrices as well as information on the algorithm used in each phylogenetic study. The phylogenetic study is central to the TreeBASE data model, as it represents the original publication details of the study, including the abstract. Despite the intrinsic taxonomic content, the developers of TreeBASE purposely excluded taxonomy (Morell, 1996). Except for the taxon names used within the trees and matrices there is no specific taxonomic scheme used. The names are not checked against or linked into any taxonomic schemes or classification. Since the inclusion of a single taxonomic scheme would not have been sufficient, and that no systems like uBio or Sp2000 existed at the time of development, it is easy to understand why the developers made this decision. The consequences however, are that the system can not support taxonomic queries.

1.5 Motivation

The TreeBASE interface (www.treebase.org) supports six query types: author, citation, study accession number, matrix accession number, taxon and structure. The taxon search, however, does not perform adequately. This search option does not effectively support higher taxa queries or synonym and vernacular queries. From a biologist's perspective, the taxon search option does not return the expected results. The query term “Aves” currently returns 5 studies (S281, S880, S296, S1166, S433). On closer inspection, there are many more studies containing Aves (birds) within TreeBASE, for example the search term *Gallus* returns a further 2 studies (S1522, S606) and *Diomedea* returns 1 more study (S351). Similarly, the search term *Puffinus* returns no studies, however, using the search terms *Puffinus tenuirostris* or *Puffinus gravis*, the study S714 in which they are located is returned. The species *Puffinus gravis* is also contained in the study S351, however, a search using the taxon name is not successful because the species text is “Puffinus gravis U74354”. These examples show that higher taxa terms, such as Aves and *Puffinus*, are not being expanded to include the scientific names contained within them. Queries performed on TreeBASE return only data where the search term matches exactly a term contained in the study. As such, the term “birds”, which is the vernacular associated with Aves, returns no data because it is not contained in any study. The synonym for *Phoebastria albatrus*, *Diomedea albatrus*, does not return the study S714 in which the currently accepted valid name exists. The taxonomic content and structure of TreeBASE does not support these queries, as query terms are not expanded to include associated terms and as a result incomplete results are returned. The current data retrieval options within TreeBASE pose a problem for the research community who commonly use taxonomic names as search terms. The research hypothesis studied in this thesis is that data retrieval through TreeBASE can be improved by the inclusion of a taxonomic infrastructure.

The taxonomic queries that TreeBASE should support are: 1) search terms should expand to include subordinate terms in the classification if they are higher taxa, 2) vernacular queries should be supported and expand appropriately to include the data linked to the scientific names, and 3) any given query should also expand to include data associated with synonyms and out of date usage of a taxon name. These queries are currently not supported by TreeBASE. The developers of TreeBASE purposely excluded taxonomy (Morell, 1996) because there were too many difficulties for a small development team to overcome. The inclusion of a taxonomic infrastructure still poses several challenges. The distributed nature of taxon names and the many data sources in which these are held is a significant problem, as few sources cover the breadth of taxonomic coverage required by TreeBASE. Also, each taxonomic data source uses a particular classification scheme supporting specific taxonomic opinions. Not only do data sources differ in the content they deliver but, even those with similar content may follow different taxonomic opinions and therefore deliver very different classification schemes.

These challenges may be addressed by combining the content of multiple taxonomic data sources and uniting the data into a form that will enable the taxon query types given above. TCl-Db, Taxonomy and Classification Database was developed to increase the accessibility and transparency of taxonomic data by integrating data from the available data sources. It was designed to provide a taxonomic infrastructure to TreeBASE and the queries systematists wish to perform.

1.6 Thesis Structure

This thesis is organised into eight chapters. The following chapter, Chapter 2, provides background on taxonomy. It explains what taxonomic data is, presents the databases that contain taxonomic data and shows how these databases are used to store taxonomic data. Following this we discuss the structure and query capacity of TreeBASE. We show, through some examples, its limited use when queried using taxon names. This leads on to the motivation for this work and the proposed data integration solution. There is an outline of data integration approaches and the general benefits offered through integrating taxonomic data.

Chapter 3 gives a full description of the design and implementation TCl-Db, the data warehouse built as a taxonomic infrastructure for TreeBASE. This chapter gives a discussion of the requirements of the database through an analysis of the currently available taxonomic databases and their ability to support taxonomic queries through TreeBASE.

The data sources and their load procedures are outlined in Chapter 4. Each data source is copied into a local silo, the schema are mapped, and the data transferred using materialized views and PL/SQL procedures.

Chapter 5 provides an overview of the queries that are supported by TCl-Db and how these can be invoked from a user interface. A web interface, a SOAP service and some of the tools created to support the use of TCl-Db data warehouse are then described. The chapter also describes a wrapper which accesses a local version of TreeBASE. The wrapper is written in PHP and uses TCl-Db to translate taxon queries into specific search terms in TreeBASE. This wrapper exemplifies the queries that TCl-Db was designed to support and the requirements of a taxonomically intelligent TreeBASE.

Chapter 6 exemplifies how this type of data integration enables data sources to be compared side by side. In this Chapter we describe how TCl-Db was used to compare taxonomic data sources with regard to both data composition and distribution. These comparisons enabled us to enhance the integration by creating links across taxon names that are related.

In Chapter 7 we demonstrate the data retrieval problems experienced by TreeBASE users through an analysis of the query logs from the TreeBASE website. We are able to show that data retrieval difficulties are in part due to the lack of taxonomic intelligence in TreeBASE, and we demonstrate the improved data retrieval based on the use of TCl-Db and the software infrastructure we have created.

Finally, Chapter 8 provides a discussion of the work presented and some thoughts and preliminary results from an alternative integration solution, using semantic web technologies. There is an outline of improvements that could be made to the data model and the user interface. Finally, an outline of further work is proposed.

Chapter 2

Background

In the previous Chapter, an introduction and an overview of the background to this thesis were provided. This Chapter explains the background in more detail. It discusses issues related to the use of scientific names, synonyms and homonyms, and classifications. It then provides details of the taxonomic databases and data sources used in this work. Then it expands on the user requirements in taxonomy and systematics and provides a high level introduction to data integration methods. This explains why the warehousing technique was selected for this work, which leads into Chapter 3 which will describe in detail the database techniques which support the user requirements.

2.1 Taxonomy

A taxonomy is a collection of terms, and a classification is the relationship among those terms. In biology, taxonomic studies involve naming and classifying organisms into a hierarchical structure representing the relationships among organisms.

Taxonomic data is the result of the processes of Naming, that is, attaching a label to a organism for the purposes of communication, and classification of organisms, which is arranging similar concepts together for the purpose of defining the logic and order of the information. The name provides a handle on the organism and the classification provides knowledge of the organism in terms of its similarity to others. These two processes are briefly outlined, and this is followed with a description of how these data are disseminated to the user community.

2.1.1 Naming

When a new organism is discovered the first thing a biologist needs to do, in order to share the discovery, is to identify the organism or name it, if it is new. Organisms are named so that they can be easily referred to in communication, publications, conversation, etc. (Jeffrey, 1989). Names are used instead of descriptive phrases since in most situations these are impractical for effective communication. For example, a geographical location is more easily communicated through a place name, a street name or number, a city name or country, or GPS co-ordinates rather than directions from place X to place Y. On the other hand, GPS co-ordinates provide more accuracy than a name, as do perhaps descriptive directions, but such levels of accuracy would be cumbersome in a conversation. It is of utmost importance that a name be unambiguous and understood by all who use it to have the same meaning. However, for taxonomic names this does not hold true, as taxon names and their organisms do not have a one to one relationship. It is fundamentally important to have clear-cut unambiguous taxon names, in order to effectively use those names.

To maintain some order in the naming and classification of organisms, taxonomists work under specific regulations, collectively called the Codes of Nomenclature. Names are managed by three main bodies, each providing policies (codes) for managing taxonomic names. These are: the International Code on Zoological Nomenclature (ICZN) (ICZN, International Commission on Zoological Nomenclature and IUBS, International Union of Biological Sciences, 1999), the International Code for Botanical Nomenclature (ICBN) (Greuter *et al.*, 1994) and the International Code of Nomenclature of Bacteria (ICNB) (Lapage, 1992). The purpose of these codes is to ensure both good working practice, through provisions that should to be followed when giving names, and to create stability of names, by ensuring that a taxon has only one scientific name by which it is properly known. In a constantly expanding knowledge base accumulated through 250 years of effort, name changes are inescapable. Even with the use of the codes, many organisms have more than one name associated with it. In order to understand why names change through time and the difficulties that arise through these changes, it is necessary to understand the practices of taxonomists and the structure of taxonomic data.

2.1.2 Scientific names

Every organism is given a name by which it is formally known, this is its scientific name. Scientific names use Latin alphabet and grammar, as in most proper names the first letter is capitalised. Taxa are organised into ranks of increasing inclusiveness (Figure 2.1) by the process of classification (grouping like with like into the same groups). The top most rank, the most inclusive, is kingdom which contains progressively less inclusive ranks to the least inclusive rank -species. The ranks genus and above, known collectively as “higher taxa”, are single terms or uninomials, while the rank species consist of two terms and is therefore a binomial. The first part of the binomial comes from the genus rank in which the species has been placed, and the second term is a specific term given to each species within the genus, the two together refer to a species. There are several ranks below species, not shown in Figure 2.1. Subspecies are

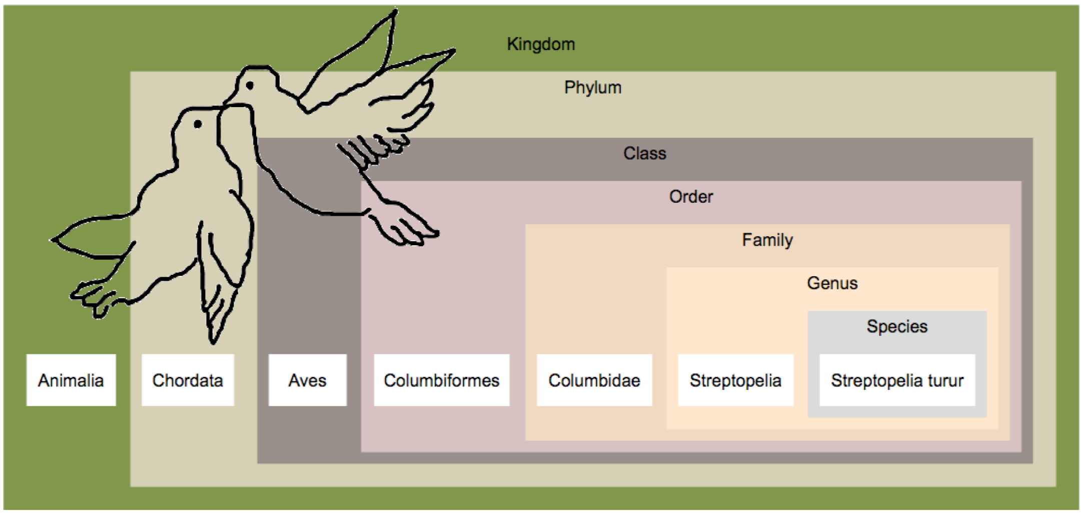


Figure 2.1: Classification of turtle doves *Streptopelia turtur*.

generally recognised as trinomials, i.e., the species binomial followed by a third term specific to the subspecies.

The different codes recognise different ranks, those that are generally accepted are shown in Figure 2.1, however, while the Zoological Code recognises the rank superfamily, the Botanical and the Bacteriological codes do not and the Botanical code uses many more ranks (variety, subvariety, form and subform) below species than any other code. The names of higher taxa ranks are given specified endings to allow them to be easily identified to a rank, a list is given in Table 2.1. This table also shows that the codes show differences in accepted endings. Other nuances across the codes include, for example, the bacteriological code only recommends that the rank should be inserted within the subspecies name as in, *Yersinia pseudotuberculosis* *subsp. pestis* whereas the botanical code insists that rank should be indicated in all ranks below species. These differences are due to the independence of the codes, they operate autonomously attending only the user community they serve.

As stated above, a taxon name is not a simple name and has two roles. A name relates not only to a taxon but also indicates to users the rank or taxonomic position of that taxon (by name endings if uninominal, lower rank if it is not). This duality (Thiele & Yeates, 2002) of taxon names is incredibly powerful as the names give both meaning and context to users. However, this duality has significant negative impacts on the data in terms of stability and change. Taxon names should clearly identify a single taxonomic concept but the process of both naming and classifying organisms in one term causes difficulty when changes and additions are made. The process of naming the world's biodiversity is far from complete (Dubois, 2003), new organisms are discovered, their names added, new knowledge of their inter-relationships is obtained and relating these to the existing structure has a considerable effect on the data. The taxonomic hierarchy organises knowledge but, as is the case for all hierarchical structures, it is not particularly good at dealing with change. In the simplest example, two organisms placed in two separate genera may at a later date, based on new knowledge, be found to be more similar than originally understood, resulting in the two genera being clumped together. Since species names use both the genus and species epithet, this results in name changes for many of the concepts originally named in the two genera. When such changes occur at higher taxa ranks, the changes cascade down and affects all levels of the hierarchy below it. It is therefore difficult to unambiguously use taxonomic names to identify taxa.

The criteria by which taxa are defined (classified) can change, for example when new organisms are discovered. The circumscription of taxonomic ranks is not strictly defined as there are no definitive criteria that are used in the assignment of a taxon to a rank. It is up to the taxonomists to make sure that the placement of the newly discovered organism exhibits only those group defining features in which it is being placed. However, those group-defining features may be called into question with new discoveries. Different expert taxonomists disagree on what defines these groups and which criteria are important in circumscription of taxa. The addition of new data may result in the addition of new ranks, a change in circumscription may result in the combining of a rank or sometimes splitting of ranks. When there are classification changes at least one taxon will undergo a change of name. In some cases the names do not change but the circumscription of the group changes. When a change in classification is made

Rank	ICBN (Botanical) (non-fungal green plants / algae / fungi)	ICNB (Bacterial)	ICZN (Zoological)
Division	(-phyta / /-mycota)		
Subdivision	(-phytina / /-mycotina)		
Class	(-opsida/ -phyceae / -mycetes)		
Subclass	(-idae / -phycidae / -mycetidae)		
Order	-ales	-ales	
Suborder	-inae	-inae	
Superfamily			(-oidea)
Family	-aceae	-aceae	-idae
Subfamily	-oideae	-oideae	-inae
Tribe	-eae	-eae	(-ini)
Subtribe	-inae	-inae	

Table 2.1: Standardised suffixes for higher taxa. Recommended suffixes are enclosed in parentheses. The different suffixes recommended for non-fungal plants are given first, followed by the algae recommendation, and the fungi recommendation. (Jeffrey, 1989)

and a new name is applied, the new name is deemed valid (or accepted) and the original name is relegated a synonym.

2.1.3 Synonyms and Homonyms

Synonyms are usually the result of name changes, the reasons for the change are either taxonomic (rank change as described above) or nomenclatural. Nomenclatural changes tend to have a more pronounced effect. For example, if a name is given to an organism by an author who does not have the knowledge that the name is already in use, the codes stipulate, that the earlier published name has priority and the newer use of the name does not apply and should change.

Name changes are common, and experts and researchers with everyday access to this data can grasp these changes and absorb the knock on effects on the hierarchy with ease. However, these effects are not easily disseminated to other research communities (Froese *et al.*, 1990). Information in the literature may be recorded under a name that is no longer deemed valid. The utility of all taxon names is in the biological information they convey and since taxon names are used as keys to their information (Geoffroy, 2001), this information becomes obscured through name changes.

Another naming anomaly results from the independence of the codes and the disparate nature of taxonomic study. Homonyms are the result of the same name (with the same spelling) being applied to different taxon concepts, often seen in botany and zoology. Article 1.4 of the zoological code explicitly stipulates that:

> Article 1.4 Independence
>
> "(T)he name of an animal taxon is not to be rejected merely because it is identical with the name of a taxon that is not an animal."

Without clear context the use of a name that refers to two different organisms can result in confusion. Again, while experts are well placed to deal with such anomalies, a non expert could get confused when using one term and finding two sets of different data. For example, using the term Morus to retrieve data will result in both Plant and Animal data returned, since this *genus* is used in both the animal and plant kingdoms.

While stability of taxon names is a particular issue in the field, an issue that needs to be addressed is the access to data associated with names that are in common use but no longer regarded by the specialists as the proper name. The resulting gap in knowledge and the potential loss of data can have significant side-effects across several fields of biology that use taxon names as information retrieval keys in their studies (Mallet & Willmott, 2003).

2.1.4 Classification

Taxonomists build their classification on a set of criteria. These criteria should group similar with similar, however, the choice of criteria used is subjective, and it is up to the taxonomist which characteristics are used for classification. Therefore, different taxonomists can place emphasis on different criteria, that attempts to best reflect the similarities and differences between the organisms. The result is multiple overlapping classifications and the same name having different meanings (circumscriptions) in different classifications. Similarly, when molecular data are used for classification these do not always agree with classifications based on morphological data (Hedges & Sibley, 1994). The classification assigns taxa to other taxa of higher ranks (depicted in Figure 2.1), and, as stated, this is generally regarded as grouping similar organisms together. Nowadays, this has shifted towards evolution (Ereshefsky, 2001; Franz, 2005), in which the systematics community group organisms by ancestry. These two forms of grouping and the resultant classifications are very different.

In biological taxonomy the classification is a containment hierarchy. The organisational criterion (Knox, 1998) in a containment hierarchy is that entities at the higher rank are composed of (or contain) entities at the next lower rank. For example, species which show some common defining feature are grouped into a more inclusive rank of genus, these are in turn grouped into families and so on. This is distinct from a phylogeny which orders entities according to their hierarchical ancestor/descendant relations. Although structured similarly (directed graphs) and similar methods for determination are used, an ancestor descendant hierarchy is distinct from a classification hierarchy in the organisation criterion of derivation (the evolutionary process being mapped) rather than inclusiveness. Ancestors are not contained within ancestors, therefore the phylogenetic trees produced through systematics are not the same as classifications (Knox, 1998).

There has been significant debate as to whether the use of two systems, and the resultant practice of merging the two systems, is having a detrimental effect on taxon names and the use of taxon names. The PhyloCode movement, to be discussed next, calls for the exclusive use of one system, that of ancestry, and the decommissioning of the classification system.

2.1.5 PhyloCode

The PhyloCode (de Queiroz & Gauthier, 1992) represents the movement away from Linnaean nomenclature (the current system) to phylogenetic nomenclature, in which species on a cladogram would allow the definition of names of taxa by their position in trees built from phylogenetic hypothesis. Supporters of the PhyloCode argue that current taxonomy was designed in a non evolutionary age and is therefore no longer appropriate, whereas their proposal, the PhyloCode, promises to promote clarity, uniqueness and stability in nomenclature through phylogenetic definition of taxa.

The proponents of this system argue that the organisation of the Linnaean hierarchy does not fully reflect the genealogical relationships in its classifications and the current practices of aligning classification and phylogeny are not appropriate. However, this system has sparked ferocious debate and while it has its followers, many have completely shunned the idea. Critics of the code especially dispute the claim to stability (Nixon, 2000) and the argument comes down to the definition of stability in the two camps; the stability of the name versus the stability of the definition, i.e., nomenclatural stability or taxonomic stability (Schuh, 2003). Others have recognised that there is some controversy about whether taxon names are defined (de Queiroz & Cantino, 2001) or not (Stuessy, 2001), and how they are defined in the current system (Moore, 2003). Those in favour of PhyloCode suggest that nomenclatural stability is more important, while the content of the named taxon may change as new organisms are placed into the phylogeny. The resulting nomenclatural stability would sacrifice taxonomic stability which the critics find unacceptable. Both sides have merit in their argument with one side providing a solution that copes with the inevitable change (phylogenies are hypotheses and are in constant flux as a natural consequence of increase in knowledge) and the other side who insist that such a radical and flawed proposal is not an appropriate solution. Indeed, to replace the whole system with a flawed one would cause more disruption than than the current system causes confusion.

There have since been other proposals to build stability into taxonomic data, with the registration of new names as a mandatory tenet of publication of taxonomic data (Borgen *et al.*, 1998; Bouchet, 1999; Knapp *et al.*, 20077; Patterson *et al.*, 2003; Thorne, 2003) and the development of networked and web accessible taxonomic data sources (Bisby *et al.*, 2002; Emery, 2003; Gewin, 2002; Godfray, 2002; Wilson, 2003).

2.2 Delivery of Taxonomic Knowledge

The standard mechanism for delivering new knowledge in the field of taxonomy is through publication within appropriate scientific journals. The data are also published in the form of field guides, checklists and monographs.

Checklists take the form of a catalogue in which all known species are listed. Checklists are a type of aide memoire and are usually devoted to particular groups or geographical locations for example the Sibley and Monroe Checklist of Birds (Monroe & Sibley, 1997). The information they provide is usually the species name the author or authority on that name and taxonomic classification.

Field Guides serve the purposes of users who need a quick and reliable data source to aid the identification of organisms in the field. These are generally small enough to be fit for purpose (i.e. taken out to the field) and therefore only provide enough data to allow a general identification through descriptions, photographs and illustration.

A monograph, by definition, is a more thorough treatment of a group often including a checklist and the important bibliographic references to original publications of the group that is being documented. Monographs can take any form and generally the information given varies according to the requirements of the group. A monograph on plants differs significantly from most zoological monographs. Generally however, they include illustrations of representative species, with, when appropriate, typical examples of the male and female, a thorough phylogeny of the group. Increasingly, taxonomic data are disseminated in database systems that are available on the web. These systems have increased the scope and use of taxonomic data in similar ways to the parallel field of Bioinformatics and the dissemination of data throughout its hundreds of databases.

2.3 Taxonomic Databases on the Web

There are a large number of taxonomic databases and the field of 'databasing' taxonomic data is as diverse as the data. These databases are built by institutions, taxonomists and generally those with a vested interest in taxonomic data. The different uses led different user communities to build databases to their meet specific needs. As a result, many heterogeneous databases exist within the taxonomic community.

There are over 200 taxonomic databases published or described, GBIF (2006) provides a list at *http://www.gbif.org/DataProviders/*. The databases that were studied and used in this project, especially at the outset, are described here. These databases were studied either because of their influence (uBio), their data (ITIS, NCBI) or their data model (Taxonomer (Pyle, 2004), IPNI (IPNI, 2006)). Sp2000 was examined initially to determine its suitability as an external taxonomic data source for TreeBASE. Those databases will now be described in more detail.

2.3.1 ITIS

The Integrated Taxonomic Information System (ITIS) (ITIS, 2006) is a partnership of federal agencies and organisations from the United States, Canada, and Mexico. It is primarily a taxonomic database serving data for "biota of interest to North America", though the data are curated by experts from around the world and the taxa are not limited to those native to North America. The taxonomic scope includes the ITIS classification and scientific names and common names in English, French, Spanish, and Portuguese. The data are available for download in a relational format at *http://www.itis.gov/ftp_download.html*, and the download includes an SQL script for building the table structures.

2.3.2 NCBI

The National Center for Biotechnology Information (NCBI) (Federhen et.al, 2005) built a curated set of names and a classification, originally for the databases within their Entrez system and, specifically, the Genbank sequence database. The NCBI taxonomy can now be downloaded as a separate database. The purpose of the taxonomic system within NCBI was to enable the names of organisms to be cross linked across NCBI tools and databases. The project started to clean up the haphazard taxonomic content, as many taxonomies were diverging within the sequence data bases and NCBI needed a consensus clean taxonomy within Entrez. Considerable effort went into building the taxonomy and has since been adopted by all the sequence databases. The data are provided as a database flat file dump at *ftp://ftp.ncbi.nih.gov/pub/taxonomy/*.

2.3.3 GRIN

The Germplasm Resources Information Network (GRIN) of the United States Department of Agriculture, Agricultural Research Service contains taxonomic and nomenclatural data for records of vascular plants. The scope and purpose of GRIN was to serve the taxonomic and nomenclatural needs of the (American) National GermPlasm System (NPGS). The GRIN taxonomy includes accepted names in family, genus, species and infraspecies ranks, common names, literature references and geographic distribution. The GRIN resource is provided over the web and individuals and organisations are encouraged to utilise the data, with the aim of making GRIN a standard reference for scientific names for plants. The GRIN data model has not been published however, this resource was included in this research for the rich data it provided.

2.3.4 Sp2000

Species 2000, Sp2000 (Bisby & Smith, 2000) aims to provide a “common gateway to species-based information in biological databases”. The focus of Sp2000 was to provide a complete list of species names, including synonyms in a style similar to a checklist (Bisby *et al.*, 2002). The Sp2000 project was amalgamated into SPICE (Jones *et al.*, 2000) and later evolved into the Catalogue of Life. The system design followed a loose federated architecture, where the data sources maintain autonomy. Although the architecture of Sp2000 is described as an “autonomous federated system”, the system is distributed as a CD, so some data are materialised in some way. The annual CD checklist in 2003 was distributed in Microsoft Access format. Later versions (2006) were moved to MySQL.

2.3.5 Online Checklists

Increasingly traditional checklist publications are being placed online. The Mammal Species of the World (MSOW) is an online checklist from the Smithsonian National Museum of History and was also used here purely as a data source. The checklist (Wilson & Reeder, 1993) is in its third edition, published in 2005, and the website provides this version for download in plain text files. The scope of the data is limited to description and bibliographic data for mammals. Other digitised checklists are also available for example, the Aves checklists from the early bird project (Hackett, 2003).

2.3.6 Other sources used to develop the TCl-Db data model

The following databases are not available for download. However, since they were also built as relational databases they were studied with the aim of understanding their structure.

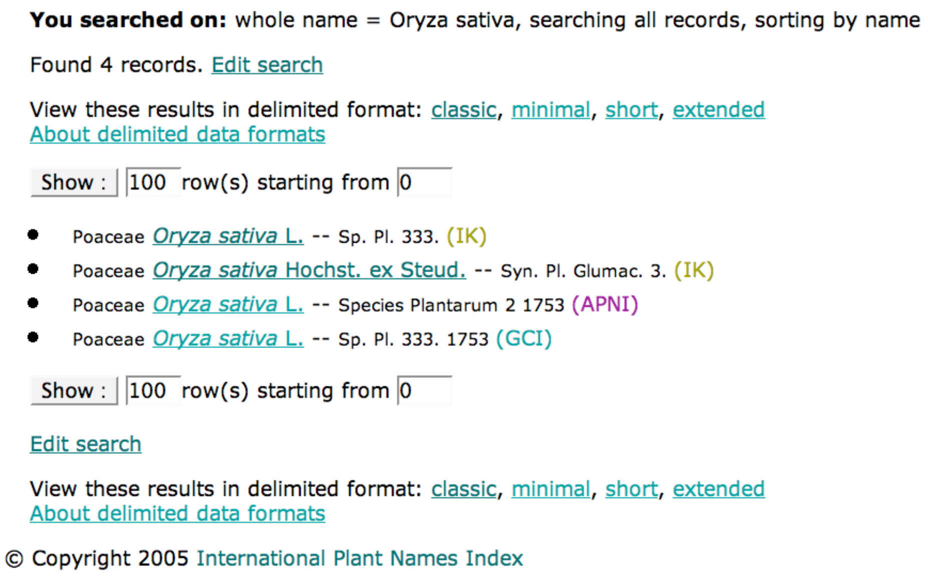
2.3.6.1 Taxonomer

Taxonomer contains a relational data model that is used to manage taxonomic names and concepts attached to specimen data at the B.P. Bishops Museum in Honolulu. The publication describing this data model (Pyle, 2004) makes very clear the distinction between a taxon name and a taxon concept. A taxonomic concept refers to a construct of a taxonomic name and its reference or the publication in which the taxonomic name is described. The taxonomer database models *Agents*, *References* and *Assertions* as taxonomic authorities, publications and taxonomic concepts respectively. The author makes use of the term ‘Protonym’ to refer to the tuple of Name OriginalAuthors(s) OriginalYear.
This tuple is a Protonym-Reference construct that is represented in the entity *Assertion.* The data model explicates the requirement of using a taxonomic concept in order to accommodate, in one database, multiple views and classifications of taxon names.

2.3.6.2 IPNI

The International Plant Name Index, IPNI (IPNI, 2006), is a database storing names for all vascular plants. The database was designed to serve as a global plant checklist. IPNI was formed as a joint venture between the Royal Botanic Gardens at Kew, the Harvard University Herbaria and the Centre for Plant Biodiversity Research in Canberra. The requirement was to improve the accessibility of internal databases at these institutions. Further, combining the limited resources for data compilation and maintenance was a strong motivation. The system has a very strong community focus, as the users contribute data and help maintain a complete index of published names.

The database has a nomenclatural focus, providing primary literature references for taxon names combined from three data sources: the Index Kewensis (IK), the Gray herbarium Card Index (GCI) and the Australian Plant Names Index (APNI) (Lughadha, 2004). The database has a central entity, the *Index Entry*, through this entity the database links to Names and the Name Authority (i.e. the author that described and published a name). There are also entities for the *Author*, *Publication* and *Source* of each *Index Entry*. Additional data in the form of Type specimens, Synonyms (and misapplied names and spelling errors) are also included in the database model. The IPNI website provides a very user friendly interface to search for taxon names, a search for the term *Oryza sativa* is shown in Figure 2.2 with each data source for the term given explicitly. The database structure of IPNI was particularly influential in this project as it provided an example of how data from multiple sources are combined into a single queriable structure.



You searched on: whole name = Oryza sativa, searching all records, sorting by name

Found 4 records. Edit search

View these results in delimited format: classic, minimal, short, extended
About delimited data formats

Show : 100 row(s) starting from 0

- Poaceae *Oryza sativa* L. -- Sp. Pl. 333. (IK)
- Poaceae *Oryza sativa* Hochst. ex Steud. -- Syn. Pl. Glumac. 3. (IK)
- Poaceae *Oryza sativa* L. -- Species Plantarum 2 1753 (APNI)
- Poaceae *Oryza sativa* L. -- Sp. Pl. 333. 1753 (GCI)

Show : 100 row(s) starting from 0

Edit search

View these results in delimited format: classic, minimal, short, extended
About delimited data formats

© Copyright 2005 International Plant Names Index

Figure 2.2: Screenshot from IPNI search on *Oryza Sativa*. Typical search results show the data that IPNI deliver, namely the taxon name including the publication in which the taxon is found.

2.3.6.3 uBio

uBio, Universal Biological Indexer and Organiser, (Patterson *et al.*, 2006) is a system that aims to gather all taxon names so that they can be indexed and used as 'metadata' terms that are capable of defining subsets of information and therefore used to retrieve information. The uBio NameBank is a biological name server, serving as a thesaurus for taxonomic names. The developers also recognised that many different names are used for the same taxon and in order for all information related to taxon to be retrieved, these names need to be linked. The remit was later extended to include classification data. ClassificationBank is a taxon concept server that stores multiple classifications and taxonomic concepts, thus extending the functionality of NameBank. This project is by far the most complete taxon name source, and is characterised by a very good API's for data access. The database structure, however, is not published, and the data are not downloadable, but only accessible through the graphical interface and the API. To some extent, uBio served as a model for the taxonomic requirements for TreeBASE, with linked names and support for multiple taxonomic opinions, however, as stated and discussed in the conclusion, the data could not be effectively linked to TreeBASE

2.3.7 Coordination across resources

The existing amalgamated databases of taxon names address some of the issues of data scope, however, these too were designed to meet particular requirements and do not support more general requirements. For example, IPNI and the International Organization For Plant Information (IOPI) database was designed to meet the requirements of a global plant checklist, Sp2000 (Bisby & Smith, 2000) extended similar requirements to all species and the uBio (uBio, 2006) name server is now both a names server and classification bank. The large number of taxonomic database systems and amalgamations have made obvious the requirements of interoperability and quality (especially in secondary amalgamated databases (Chapman, 2005a)). Encouragingly, many of the stable published databases have some affiliation to TDWG (Taxonomic Databases Working Group) who are beginning to address the requirements of taxonomic data across several user communities.

2.3.7.1 TDWG

TDWG and GBIF (Global Biodiversity Information facility) (Saarenmaa, 1999) have started looking at the more global requirements of taxonomic databases. TDWG's remit is specifically to build interoperability through standards and protocols. GBIF have an overlapping element but aim to use the standards output from TDWG to build tools that will enable interoperability through their network and make biodiversity data more freely accessible.

TDWG ratified and published the Taxonomic Concept Schema (TCS) in 2006. Taxonomic concepts (Franz *et al.*, 2006) are entities created to tackle the inherent problems of using names as unique identifiers, as names in different databases are not necessarily equivalent. The data associated with a name are vital to the use of that name and therefore the understanding of the name. A richer association of metadata and taxon name can address this. Taxon concepts can do this through associating the reference (the definition) of the name with the name itself as a two part entity. This two part entity enables the unique association of a taxon to its original data.

This is especially important in taxonomic information interchange. The SEEK Project (SEEK, 2006), where the TCS was originally conceived, is reaching out to the data concerns of ecologists and the TCS was originally designed to enable data integration across ecological data sources. Integrating data from two databases by matching purely on the taxon name can result in significant loss of information. Ecologists require a certain amount of precision in the data they use and therefore require stringent taxonomic data co-ordination. Moving a taxon name from one database to another purely based on the name string would for example, result in the loss of information pertaining to the taxonomic position in the hierarchy (if the two systems used different classification schemes), or to specimen information (if the two systems came from different geographic locations). A mechanism was required to transmit data across systems while retaining the uniqueness of the taxon in the individual systems, within the integrated data. Such metadata (literature reference, rank and taxonomic position, specimens) enable better understanding of the name concept in the data systems and therefore of the meaning of the taxon.

Using the TCS with the additional metadata, information can be transferred without ambiguity and the loss of meaning from the original data provider. The integrated data can be linked without confusion backwards to the original data sources through this scheme. See references; Kennedy *et al.* (2005); Franz (2006); Berendsohn (1995) and Gradstein *et al.* (2001).

The limitations, however, are the number of taxonomic data sources that have enough data to fully utilise the TCS. The systems most likely to contain such verbose data will be at herbariums and museums (primary data sources) that have links to literature references and specimen references. Considerable effort is also required to adapt data in this format for transfer (mapping two relational database schemas is much simpler). Although the majority of components are optional within the schema, its full value will only be realised when the transformation into the structure is made seamless and data is made available and openly disseminated to the community in this format. This falls into the remit of GBIF.

2.3.7.2 GBIF

GBIF focuses particularly on data about species and specimens, with appropriate links to other relevant data. The data GBIF will take responsibility for are (GBIF, 2006):

1. Taxonomic data, including
    (a) Taxon names (the responsibility of the ECAT Work Programme)
        i. Scientific names, including data on synonymy
        ii. Vernacular names
    (b) Taxonomic descriptions, including diagnostic keys
2. Taxon occurrence information (primarily species-level, but including data for taxa at different ranks where appropriate)
    (a) Specimen records (from natural history collections)
    (b) Observation records
3. Links to other taxon-level information, including
    (a) Information on taxon biology and life history
    (b) Ecological interactions
    (c) Genetic data
    (d) Sound and image resources

The Taxonomic element is the most relevant to this work and is also their initial priority. Using the TDWG ratified Taxanomic Concept Transfer Schema, GBIF have started exchanging taxonomic data across their network (the GBIF portal can be found at http://data.gbif.org/), this will take the form of ECAT (Electronic Catalogue of Names of Known Organisms), a digital listing of the names of all known species. ECAT is being developed in collaboration with Species 2000 (Bisby & Smith, 2000), ITIS (ITIS, 2006), uBio (uBio, 2006), the providers of taxonomic nomenclators, taxonomic institutions worldwide, the nomenclatural codes and others. In 2005, ECAT contained about 983,000 species names from nearly 200 data providers; it aims to have a complete listing of all known species by 2010.

2.4 Taxonomy and systematics

Despite a plethora of taxonomic databases, there is no database of taxonomic names that has been developed specifically for the tree building community, and no taxonomic database currently meets the requirements of this community. This is perhaps difficult to fathom given the interdependence of taxonomy and systematics. The reasons for this are highlighted here.

Uniquely, systematists are both taxonomic users and taxonomic data providers through building the phylogenies on which classifications are based. As such, they have unique taxonomic requirements and often visit many taxonomic data sources, compared to taxonomists whose needs are met by one or perhaps two systems. Taxonomists, generally work on small groups of organisms and they focus more narrowly sometimes on geographical locations or geological time periods. Getting a handle on other data, even for an expert, when not actively involved in the research, can be difficult. This is partly due to the complications associated with taxonomic data as described above (synonyms, name changes and taxonomic revisions), but also because of the data accessibility, particularly moving from one database system to another. There are many taxonomic database systems and they each have a very specific data scope and were usually built for a specific user community. Prometheus (Pullan *et al.*, 2000), for example, although extensible, has a working data scope of plants and was built to manage these data through the working practices of taxonomists. There are also many examples of literature and specimen databases that have taxonomic content but are not taxonomic databases. In these cases, the interfaces to these systems are designed with particular queries in mind, and using them outside of the original scope, say to extract all taxonomic data, can be difficult and sometimes impossible through the interfaces provided. Although, some database have been built to expressly index names so that they can be used to retrieve data (Berendsohn, 2003), the focus was towards retrieving literature data. Databases that performed literature retrieval well, with the exception of uBio, had limited data scope. Given that no system has been designed with the data scope and query interface geared towards the systematics community, currently systematists have to visit and learn to use many systems and from these gather the data they require and collate and manipulate it into a form they can use.

2.4.1 TreeBASE

TreeBASE Morell (1996) is a phylogenetic and evolutionary information store now containing phylogenies for more than 90,000 taxa. Despite the intrinsic taxonomic content, at design, the developers of TreeBASE purposely excluded taxonomy. This decision was taken because at the time of development, there were few electronic taxonomic data sources to choose from and there was also the question of which classification to use. This is still an issue. As we show in Chapter 5 names in different classifications can have different meanings hierarchically, for example, Aves in NCBI and Aves in ITIS are quite different in their data coverage and content. Also, some classifications do not support some commonly used ranks and data coverage varies across the taxonomic data sources. It would be unfitting to apply one single classification to TreeBASE, but without a classification, TreeBASE does not effectively support higher taxa queries.

Currently, data can only be retrieved by exact of partial string matching. As a result, systematists prefer to gather the data they require for their analysis through literature searches. In most cases, once data are retrieved the search results have to be manually examined to determine if they contain the phylogenetic data of interest. The lack of taxonomic intelligence makes data retrieval through TreeBASE difficult. Currently, in order to retrieve all bird sequences a user would first have to find all the scientific names and any synonyms he is interested in and then perform the searches one at a time using this list. It would be far more efficient if the query term "birds" translated to Aves which, in turn translated hierarchically by the system, this is what is meant by 'taxonomic intelligence'.

2.4.2 TreeBASE Database versus Information Retrieval

When querying a database system, the results returned are exactly those data that satisfy the given query. This is referred to as data retrieval and in relational database systems it can be accomplished by the structured query language (SQL). For effective data retrieval, the data has well defined structure and should have well defined semantics. A well formed query will return exactly those data that satisfy that query. In information retrieval, ideally, a given query is understood by the system, i.e., there is an element of interpretation through related terms or categorised topics (Fast *et al.*, 2002). The query therefore does not have to be exact and the data returned is not that which matches the query but that which is *relevant to the query.* The query need neither be well formed nor exact.

The queries supported by the TreeBASE interface do not perform adequately, as it does not support higher taxa queries or synonym and vernacular queries. Currently TreeBASE provides only data retrieval capacity, (as outlined in Section 1.5) and as we show in Chapter 7, in the searches performed on TreeBASE, the users expect information retrieval, which means that the systems does not perform as expected.

2.4.3 Requirements of a "Taxonomically Aware" Database

At the very least, the taxonomic requirements that TreeBASE should support are:

- search terms should expand to include subordinate terms in the classification if they are higher taxa

- vernacular queries should be supported and expand appropriately to include the data linked to the scientific names

- any given query should also expand to include data associated with synonyms and out of date usage of a taxon name

2.4.3.1 Support for Hierarchical Query Expansion

Genbank (Wheeler *et al.*, 2007) is an example of a database with a taxonomic intelligence. Each sequence record in Genbank includes the data; the organism name and organism classification. By using this information queries such as 'select all Insecta sequences', 'select all plant sequences' or 'select all sequences in the genus *Drosophilla*' retrieve the data in a taxonomically intelligent manner, i.e. by resolving the query hierarchically. This is what users expect when they perform a query using a higher taxa search term and is what a taxonomically aware database should be able to achieve. TreeBASE was built when there were few taxonomic databases available. While NCBI had the resources to build the taxonomy (Federhen et.al, 2005) they required for information retrieval, smaller projects such as TreeBASE, due to financial constraints, could achieve the same. The Genbank model highlights the requirements of taxonomic intelligence that would potentially make TreeBASE a more attractive information provider.

Many queries that users perform are higher taxa queries. As data are often collected for multiple taxa, it is easier to use the higher taxa that include all the species of interest, than it is to search for each species name individually. Higher taxa queries implicitly include all lower taxa in the hierarchy, and as a result make the queries more succinct and easier to formulate. Including hierarchical queries in TreeBASE can be easily achieved with the inclusion of the NCBI taxonomy. However, the difficulty here is that NCBI provides just one taxonomic view and there are multiple overlapping classifications which may be useful in different user communities. Some users may wish to use higher taxa groups that are not contained in the NCBI classification. This poses a problem for systems such as TreeBASE that store data across classifications, and the storage of these classifications and the choice of which classification to traverse when performing these hierarchical queries is a significant consideration. In this respect, Genbank only provides one particular view of taxonomy, and no others, which may not be suitable for all TreeBASE users.

2.4.3.2 Query Expansion with Synonyms and Vernaculars

It seems that users prefer to perform loose queries in the hope of gathering all the data (and not loose anything of value) and manually filter the result set. Vernaculars can be considered to be loose queries, for example, a cat could refer to all species in the family Felidae, where as puma, cougar and mountain lion have a little more specificity. The use of loose search terms is typical in a "drill down" search, which is usually performed when a user has a rough idea of what she is looking for but is not exactly sure, and chooses to browse the relevant data until she comes across the actual search term. The use of loose query terms is similar to hierarchical query expansion, in that the query term should also translate from the vernacular to the currently accepted scientific name. Indeed, judging from the queries we examined (see Chapter 7), a user expects that the query translates to the scientific name and any other synonyms and vernaculars that are linked to that scientific name.

Synonyms are not loose queries but queries that are performed either because the user knows exactly what she is looking for or because she is unaware of the current status of the name and is using it in error. This should not cripple a user in their search strategy, and similarly, synonyms should translate in much the same way as vernaculars, so that all *relevant* data are returned to the user, despite the fact that the user provided a very specific query term.

2.4.3.3 Consistency

Consistent use of names is important in information retrieval. If the database system only allows the use of a single name for a given concept, the data linked to that name can be retrieved when using the name as a search term. However, if names are used inconsistently, i.e. with two different spellings, then some data will be attached to one use of the name and some other data to the other spelling (Rothschild, 1989). In order to get all data of interest, both names would have to be used as the search term. However, two different classification schemes may rightly or wrongly use different spellings, i.e., the spellings Boopidae vs. Boopiidae shown in

Figure 2.3. It is therefore an important design consideration to allow mismatches in search terms as taxonomic names take Latin form and the exact spelling can sometimes be difficult to decipher for both experts and novices. As a result, spelling mistakes have propagated through the data. Not only do users require some capacity to check for the correct spelling of a name but they should also be able to retrieve data that has been used with an alternative spelling. An approximate string match tool can be employed that will enable the system to find a match even if a query it is misspelt.

2.4.3.4 Data Coverage

Simply employing the NCBI taxonomy, as used in Genbank, is not a solution to all the taxonomic requirements of TreeBASE or the work of all systematists. In some cases, there is an obvious choice of a taxonomic data source, however, there are cases where users require full coverage of all known named organisms. In the example, in Figure 2.3 we see that Genbank is not a complete source of taxonomic data for lice. Many more taxon names can usually be found in the classifications of constructed by experts. In Genbank the sarch term Aves returns 4645 taxon names while the same search in ITIS returns 14,095 names. Considering this, the NCBI taxonomy alone would not suffice for the working practices of systematists. Most researchers in the field are able to find with ease the most up-to-date checklist on particular groups, however, these checklists are not always linked to data. For example, 4645 bird names are linked to a sequence, but names in stand alone checklists are not digitally linked to data. Using another taxonomic scheme requires manually synonymising names across the schemes in order to translate the query term in one, to the relevant query term in the other. For example, Charadii vs Charadiiformes is a required synonymisation. It is therefore important for a taxonomy database to provide full coverage of the estimated 1.7 million known species (Alroy, 2002) by including as many taxonomic data sources as possible.

These challenges may be addressed by combining the content of multiple taxonomic data sources and integrating the data into a form that can support taxon queries in TreeBASE. The research hypothesis studied in this project is that data retrieval from TreeBASE can be improved by the inclusion of a taxonomic infrastructure. This infrastructure must provide a wide coverage of data and therefore a merged, integrated view of taxonomic data through a single point of access is required.

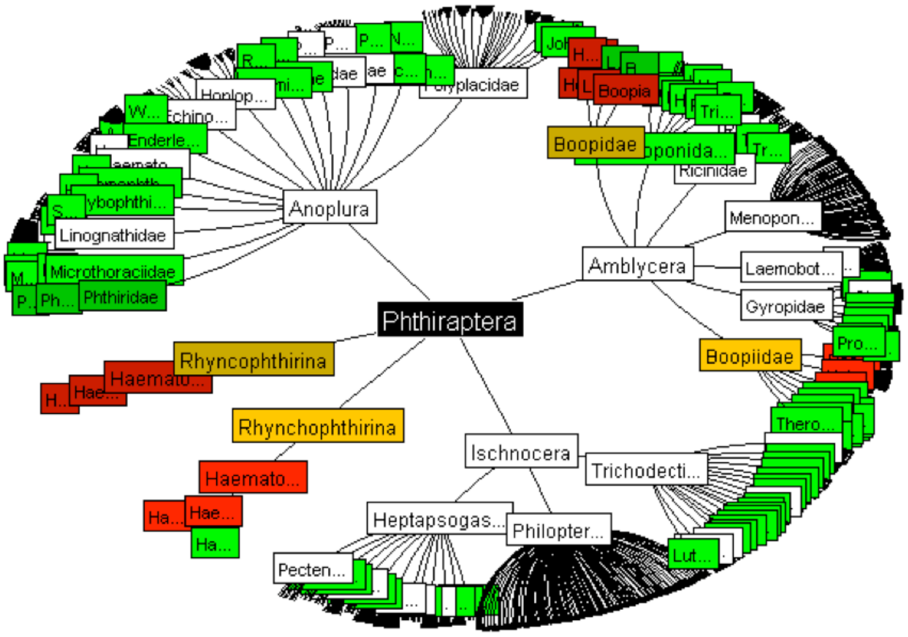


Figure 2.3: A comparison of two different classifications of Lice shown using an applet (Grant, 2004). A classification provided by Vince Smith, currently at the Natural History Museum, London and the NCBI classification starting from the node Phthiraptera. The colour assignment is as follows:
Black = The root of the tree (top level of classification),
White = Nodes that are the same in both trees,
Green = Nodes that occur only in one of the trees,
Red = Nodes that have the same name but are classified differently in the two trees,
Orange =The point at which the classifications of the red nodes diverge.
The red nodes highlight the classification differences, this is because Rhyncophthirina and Rhynchophthirinia and Boopidae and Boopiidae are spelt differently in the two classifications. The darker shades of these colour represent nodes in the NCBI classification. The number of light green nodes indicates that the Vince Smith classification has far greater data coverage than the NCBI classification. This data was part of a masters project carried out by E. Grant, see `http://www.dcs.gla.ac.uk/~grantej/treebolic/DATA/liceTaxonomy.html`.

2.5 Integration approaches and database technologies

It is clear from the taxonomic requirements of TreeBASE that a taxonomic database is required that can deliver a broad coverage of taxa and multiple classifications. The proposed approach is to build this database specifically for TreeBASE. A database is defined as a collection of related information about a subject, organised into a useful manner that allows the data to be safely stored, accessed and analysed. This section briefly outlines database technologies that are in prominent use in biology.

2.5.1 Database technologies

Database System

The term database system (or more accurately database management system) is distinct from database, although the terms are used synonymously. A database system comprises the computer programs used to manage and query a database, while databases are structured collections of related data. The structure of the data is the key component of a database, and is modelled by the database schema. A database schema represents the structural description of the data that is held and the objects and relationships among them. There are different ways of organising a database schema. The different database models that are in use described below.

Database management systems are categorised by the data model they support. The relational model is the most commonly used. Object Relational is a relatively recent addition and there are the older Hierarchical and Network Models. The database system also provides a language to access the data. These two components of a DBMS, the model supported and the query language, are a key part of the decision for which system to use in the development of a database. One other data model that is not supported by any particular management system[1] is the flat model.

Flat files

In the early days of computing (when magnetic tapes/punch cards were in widespread use) data was generally structured in a flat model. This data model represented data in simple files of sequential records. The more commonly used term now is "flat file" since they are distinct from most other data models and this term is more literal. In a flat file one record is sequentially followed by the next, and the file contains only data and delimiters. The field delimiters and

[1]Excluding the operating system - these were essentially filesystems similar to those currently in use.

the record delimiters are commonly commas and newlines. Fixed width flat files were the first implementations where the fields were padded (with spaces) to a particular width[2]. Flat files are still common data structures. They are simple tables (precursor to spreadsheets), easy to use and conceptualise and one of the main reasons they have stayed in regular use is that they are easy to share and transform into other structures.

With the ease of use came several limitations, in particular the operations on these structures were limited to: opening the file and reading the current record and only basic operations to allow you to go to the next, first, last, previous or *n*th record with only insert, update and delete manipulations. These file systems were soon found to be lacking as a database, given the overhead of opening and closing files, the problems associated with redundant data[3] and concurrent access [4]. In terms of data management, flat files were especially inappropriate for complex data.

Though flat files are making a revival through more sophisticated structured XML files, other data models offer more adequate solutions to databases and data management.

Hierarchical Model

The first data model in prominent use was the Hierarchical model. In this model data is structured as a tree (hierarchy), similar to the taxonomic tree structure. Data at each level in the hierarchy are either related or dependant upon data at the level higher. The model presents data as RECORDS, records have FIELDS and the FIELDS hold the DATA VALUES. RECORDS are connected to each other through LINKS, and LINKS connect two records.

However, while the hierarchical model is very fast and efficient at querying hierarchies, certain queries can be difficult, i.e. querying across multiple trees. Also, these models are not designed for regularly changing hierarchies. The most widely used hierarchical DBMS is IBM's IMS (Information Management System) (Strickland *et al.*, 1982), initially developed for the Apollo space program back in the 1960's and still in use today in many financial systems. However, it runs only on IBM's mainframe hardware and is integrally linked to the Z/OS operating system making it an inaccessible product for most academic environments.

A newer Linux-based and open source implementation called Mumps/MDH (The Multi-Dimensional and Hierarchical Database Toolkit (O'Kane, 2006)) provides hierarchical storage and retrieval and has been shown to work very well. It has been implemented successfully for

[2]80 digit punch cards are an example of fixed width flat file.
[3]the same data in many files
[4]data corruption through two processes attempting to modify the same data file

large genome data sets (O'Kane & Lockner, 2004) with added functions including Perl regular expressions, string searching algorithms and the Smith-Waterman alignment algorithm. This is one of many Mumps based information systems which are mostly implemented in the healthcare industry, MDH is perhaps the first implementation within the bioinformatics community. However, Mumps is a rather esoteric programming language, pre-dating many of those currently in use today and therefore has a very different syntax. The MDH implementation supports access to the PostgreSQL DBMS, the Perl Compatible Regular Expression Library, the Berkeley Data Base. The database with its functions is available as C++ classes, making it the most accessible Mumps implementation so far and may prove more popular in the future.

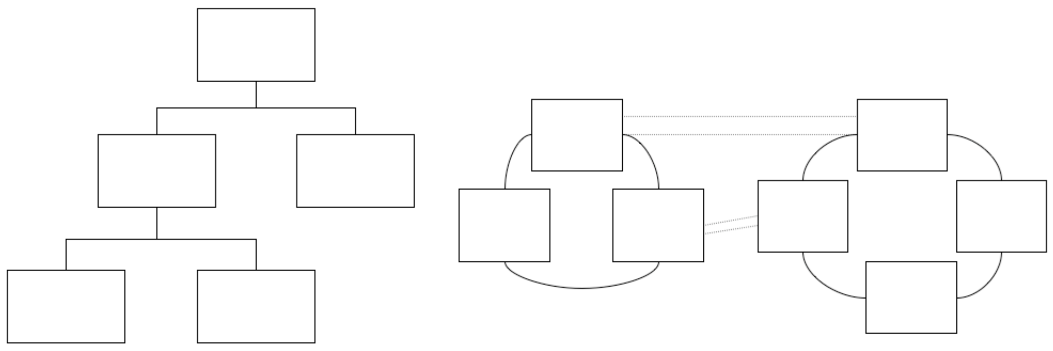


Figure 2.4: Hierarchical Model on the the left and the Network Model on the right. Adapted from Greenwald *et al.* (1999) Figure 1-1.

The hierarchical model allows 1:N (one to many) relationships between RECORDS, i.e. a record (the parent) can have many children records, the children can have only one parent. To enable multiple parent-child relationships (N:N or many to many), the Network model was established. The network model differs from the hierarchical model in that the hierarchical model must form a tree structure while a network model allows arbitrary graphs. The model is record based. Records in the network model are a collection of data items. Records grouped together are SET TYPES. CODASYL (Conference On DAta SYstems Languages) (Taylor & Frank, 1976) formally defined the network model in 1971, it is based on mathematical set theory, where a set defines the 1:N, N:N and also 1:1 relationships. Figure 2.4 gives a schematic of the difference between the hierarchical and network models. The Network model however was very quickly displaced by the Relational model.

The Relational Model

The Relational model (Codd, 1970) is by far the biggest success story in database research. Also based on mathematical set theory, its biggest advantage was in the simplification of systems through independence of data from the application. In all the systems described above, the data and application were tightly coupled. In the relational model this is not so, because the data model and implementation (physical components that constitute the model) are distinct and 'data independence' is achieved. What this means to application designers is that if changes are made to the way the data are stored and accessed at the physical level, no corresponding changes are needed at the application level. The way the data looks to the user and the way queries are made do not need to change.

The language of the relational system also simplified data access, as older systems commonly used procedural languages, working on one record at a time, while relational programming is non procedural working on sets. At another level of simplification, data consistency in the relational database is enforced, not by rules built into the applications but through constraints which are part of the logical schema. The same rules are accessible from the schema and they do not have to be built into each individual application that accesses the data. Overall, it was these simplifications of data management and data querying that resulted in the Relational Model dominating the database market. One other reason the relational databases grew to be more dominant was through the availability of multiple platform versions; unlike IBM's IMS, for example, the Oracle relational database was available on nearly all the early operating systems (Greenwald *et al.*, 1999). The Relational Model is the most accessible and by far the easiest to use system of all those described. It is predominant in bioinformatics and indeed most of the taxonomic databases currently available are built on a relational model.

The Object-Oriented Model

The object-oriented (OO) database model (Silberschatz *et al.*, 1996) is adapted, as the name suggests, from the object oriented paradigm used in programming languages. The model is based on objects and their relationships, contrasting them from the record based relational model. Within the OO data model, data are represented as objects. These in turn, are organised into classes, giving a hierarchical structure where classes inherit from its parent. Both data, and operations on the data (methods), are stored in the database as objects and since data values are stored as objects, objects can be shared. Using object identity, two objects can share components, other objects or methods. The hierarchical structure of classes facilitates the re-use of methods. Object-oriented models are used for systems where other data models, such as the relational model, can not be used easily to capture the underlying structure of the data.

Graph Model

The graph database models (Angles & Gutierrez, 2008) were popularised alongside OO models and were developed to explicitly capture the inherent graph structure of certain data, i.e. hypertext data. In graph databases the data structure (and the schema) are represented as graphs (directed, labelled) or a generalisation of a graph (hypernode, hypergraphs) and data manipulations are expressed as graph-oriented queries. Each of the proposed graph data models supports node labelled digraphs and the majority also support edge labels. An example schema and instance for the graph database model GOOD is presented in Figure 2.5 and the more recent model, the Graph Data Model (GDM) is presented in Figure 2.6. GDM was based on the GOOD data-model but extended to support complex objects.

2.5.2 Data Integration

Data integration involves combining data, so that data from a number of heterogeneous data sources can be queried seamlessly. Data integration offers significant advantages to users, namely; transparency and extensibility of data. Data from several different sources often need to be queried in specific ways, by integrating the data accessibility is made efficient and differences and overlaps in the data are made more obvious. Also, in terms of extensibility, if is often difficult to use data outside of the scope provided by individual data providers, data integration offers to extend the scope of data use. Data integration is most often achieved through Database Integration.

The establishment of reliable data management solutions has resulted in increasing numbers of easily accessible information resources. However, with large number of databases built for specific needs and requirements, especially in the biological sciences, data has become more disparate and the focus has shifted towards data integration in order to maximise the use of these data. The main goal of data integration systems is to provide a mechanism to unify databases so that users do not have to manually query multiple databases and collate the results. There are clear benefits to be gained from integrating data other than the convenience

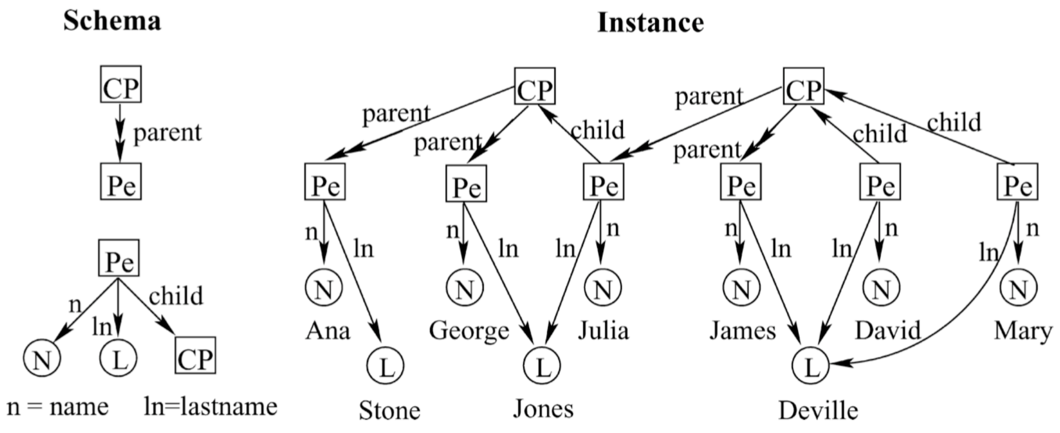


Figure 2.5: GOOD, Graph Object-Oriented Data Model taken from Angles & Gutierrez (2008) Figure 11. The schema graph on the left represent the parent child relationship through the nodes Pe (person) and CP (child-parent), the double arrowed edge between CP and Pe labelled Parent indicates a multi-valued attribute. A person has more than one parent. The child attribute of a person is indicated below with a single arrowed edge, indicating that a person can only be the child of one Child-Parent instance. For example, Person with name Julia and last name Jones is a child of the child-parent relation, which has two parents Ana Jones and George Jones.

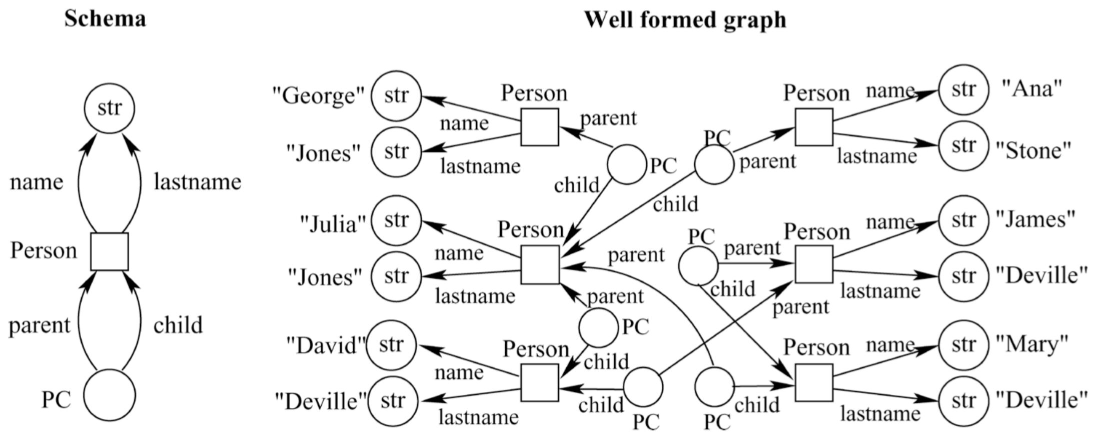


Figure 2.6: GDM, Graph Data Model taken from Angles & Gutierrez (2008) Figure 11. The schema is represented in the graph on the left, nodes are classes and the attributes are represented as edges. The Person class has attributes name and lastname. Person is an object node, PC is a composite-value node and has the attributes parent and child. Str is a basic value node, representing the values name and lastname. ‘The instance is the graph on the right. In the instance graph we see the parent child relationship between George Jones and Julia Jones represented as: Person, with name “George” and last name “Jones” is a parent and has child, a Person with name “Julia” and lastname “Jones”.

of not having to query several databases; the ability to extract data and make predictions or decisions from integrated sources is just not possible when the databases are queried in isolation.

In data integration, the data are combined from two or more databases (data sources) into one large database (Lenzerini, 2002). Within the large integrated database, the consolidated data can be queried as a unit, thus allowing more information to be acquired from the data (Calvanese *et al.*, 1999). One approach to data integration is database federation which consists of relational database that provides uniform access to two or more heterogeneous data sources. *Database federation* is an effective approach to integration of heterogeneous data sources when the data can not be materialised into the integrated database (a data warehouse). Data integration using a data warehouse approach, where data from the data sources are physically combined into one structure, is a very mature field. The data warehousing solutions (OLAP - see below) and data federation tools (query rewrite and cost-based optimisation) are well established and used in many production systems.

Through a federated approach, the combining of data from several data sources can be accomplished in several ways. In a loose federation (Figure 2.7), application systems are built to directly combine data retrieved from querying the individual data sources. These special purpose applications are often a ‘quick and dirty solution’. They are quick because integration is coded into the applications which are inexpensive and simple to build, but dirty, because these systems are expensive to maintain especially as they are easily broken by changes to the underlying sources (new data sources generally require the application to be re-written), see Figure 2.8.

More robust data integration systems generally follow a materialised approach (Figure 2.7), where the degree of federation is based on requirements and data availability. Where data are being integrated from different organisations, those organisation may choose to make the data available in such a way that the underlying data sources remain under their control. These autonomous data sources force the development towards loose federation. However, where the requirements show data mining or decision support queries then performance becomes the key driver to the degree of federation, pushing towards a data warehouse. This approach is illustrated in Figure 2.9.

In a data warehouse copies of data from several sources are stored in a single database, using a global schema (Bouzeghoub & Lenzerini, 2001). The components of a data warehouse are the sources containing the original data, the global schema providing the integrated view of the data and the data load processes that transform the data from the sources to the global schema.

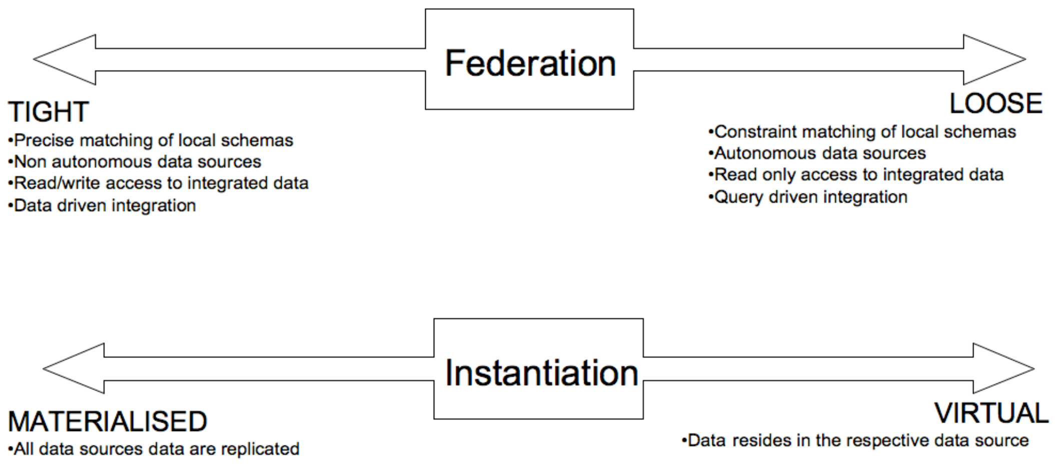

Federation
TIGHT
•Precise matching of local schemas
•Non autonomous data sources
•Read/write access to integrated data
•Data driven integration
LOOSE
•Constraint matching of local schemas
•Autonomous data sources
•Read only access to integrated data
•Query driven integration
Instantiation
MATERIALISED
•All data sources data are replicated
VIRTUAL
•Data resides in the respective data source

Figure 2.7: Degree of Federation and Instantiation in integration methodologies. Data warehouses fall to the left in the diagram above. Generally, warehouses are computationally more efficient since they provide high performance and are scalable. Loose federations have several advantages also, since the data are not replicated and the data sources can be anything from flat files, XML files to application programs (see Figure 2.9).

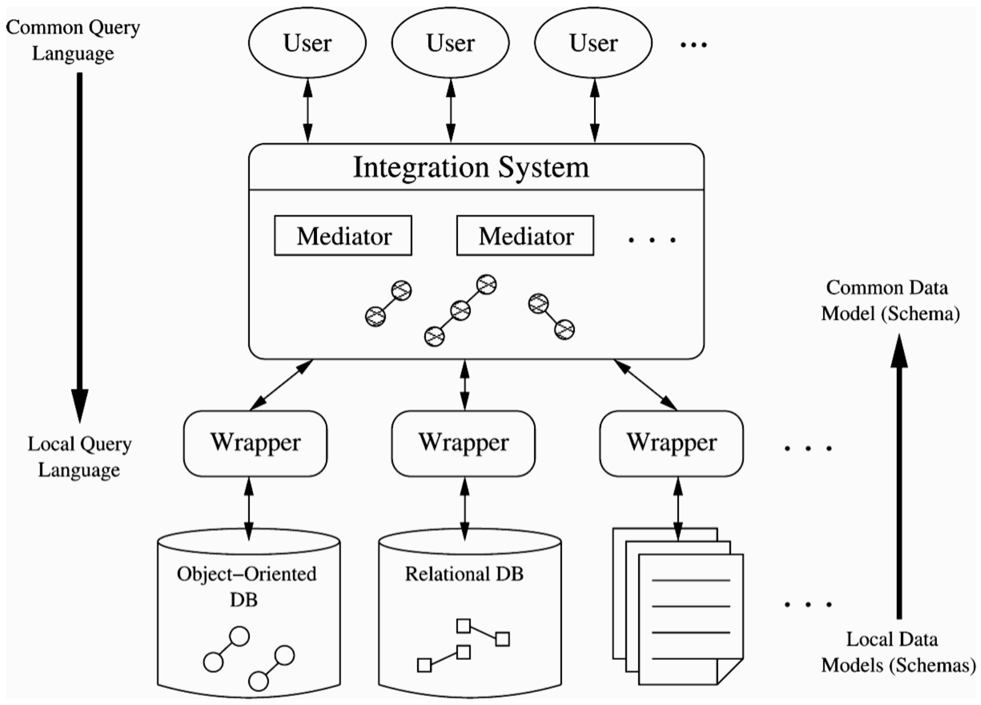


Figure 2.8: Overview of Loose Federation Procedure taken from Karasavvas *et al.* (2004). This diagram shows query driven integration. Data are extracted from the sources only when queries are posed. The integration system contains no data, the wrappers access the data sources, extract the relevant data and return those data in some specified format read by the mediator which merges the data from each wrapper and returns the integrated data to the user. The data sources remain autonomous. In a materialised federation, integration is data driven (see Figure 2.9)

During the load processes data are usually filtered or cleaned. One of the primary uses of a data warehouse is for decision support. In the commercial business sector, the need for in-depth analysis of data for determining statistical patterns of consumers, stock updates, forecasting from sale patterns, financial reporting etc., essentially drove the establishment of data warehouse technologies. The focus of analysis (complex queries) in warehouses over transactions (updates, inserts deletes) led to the development of OLAP (On-Line Analytical Processing (Chaudhuri & Dayal, 1997)). [6].

The database federation approach can form either a virtual warehouse or a materialised warehouse, depending on whether the data can be physically moved. Generally the term warehouse is synonymised with a materialised warehouse; the term warehouse is used here in reference to a materialised warehouse.

It is commonly accepted that data warehousing is the most effective way to provide the data for business decision support queries (Hoven, 1998). Data warehouses have several advantages but mainly the powerful high-level query language (SQL) greatly simplifies the combining and comparing of data, transferring data and of course all the other features of relational database management systems in terms of performance, reliability and extensibility.

There has been a notable shift in data integration more recently, since the internet has accelerated the decentralised nature of data. Many newer technologies are gaining ground especially as many data sets, due to size, are too large to physically move. Data (or information) integration is now a pivotal area of research and highlighted as one of the main uses of semantic web technologies (Berners-Lee *et al.*, 2001a).

2.5.3 Steps to Integration in Data Warehouses

In the context of a materialised data warehouse, the process can be outlined in three steps.

1. Identification of the sources and source schemata where the relevant information resides.
2. Schema Matching: mapping source schemata to the warehouse structure (global schema).
3. Data Transformation: Combining data within the data warehouse structure (global schema).

The first step involves identifying the sources where the relevant information resides and acquires the data. In most business environments these are internal data silos but in academic research these are usually public domain databases. These data are then mapped from the source data

[6]Traditional databases were OLTP systems (On-Line Transaction Processing).

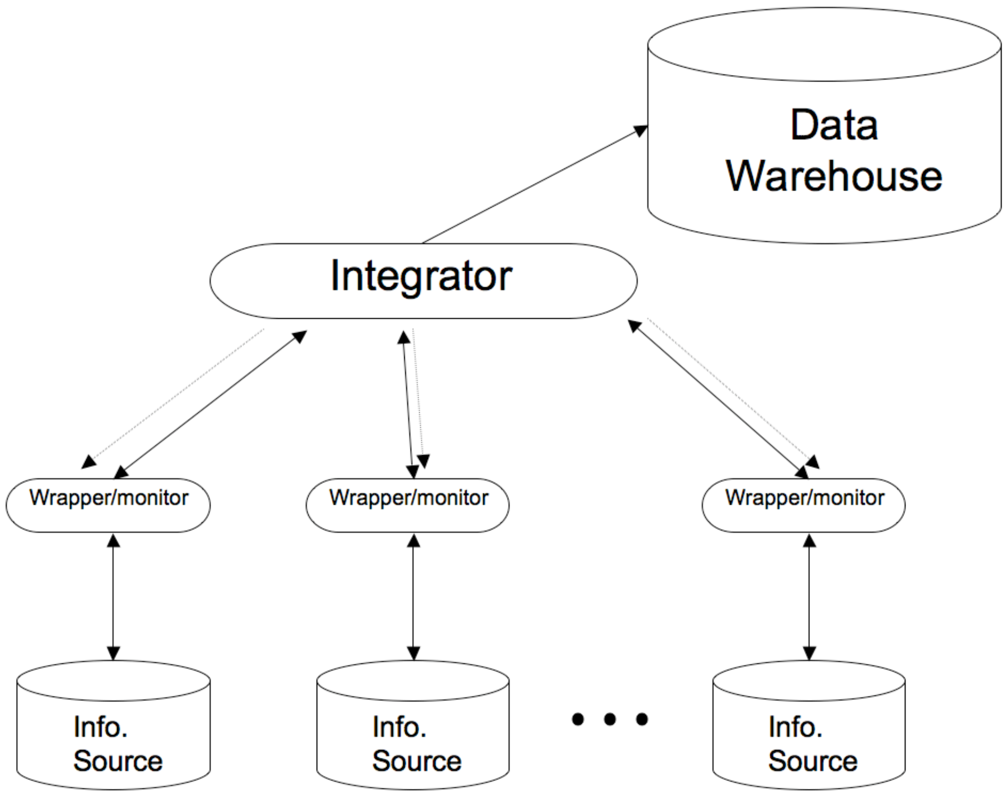


Figure 2.9: Materialised federation, Data Warehouse, taken from Widom (1995). In this methodology the integration is data driven, the data flows from the information sources at the bottom to the data warehouse at the top. The Integrator transforms the data into the data warehouse from the information sources. Monitors may be employed to check periodically for data that need to be transferred. The wrappers access the data that are to be transferred, these could be simple SQL statements or programs to retrieve the data from the sources. The diagram suggests that the information sources are databases but they need not be. Data sources can be also, XML files, flat files or Excel files.

structure (schema) to the warehouse schema (schema matching) and finally integration occurs as physical transformation of the data to the data warehouse schema. Particular attention is paid to the second step, mapping of the source schemata to the warehouse schema since this is the most challenging step in the process.

2.5.3.1 Schema Matching

Schema matching (Navathe *et al.*, 1984) is the interpretation of the data within the data sources before integration (i.e. before building the transformation code to transfer data in the source schema to the destination schema). Schemata are the structural description of the data held in data stores and as such are metadata. Some schemata also address data contents through, for example, allowable values and meaning of data through cardinality and referential integrity. As much as databases are heterogeneous, their schema representations are equally heterogeneous, making the process of mapping across schemata a manual task. The mapping process looks at data elements described in the schema to determine how and which data elements should be transformed into the source schema. An example is given in Figure 2.10, showing the mapping between two different schema structures. The first step is the comparison of the source schema to the corresponding destination/global schema. In the example given, we can map Style to Genre, Band to Artist and so on. These are semantic correspondences between the two schemata. In many cases the mapping is clear through, however, cases such as Track and Title could be tricky given only this level of metadata. Quite often it is necessary to look at data items, for example, Track could equally map to Name or Title. However, if it turned out that tracks in this case are numbers (e.g. Track 1) it would not map to any of the items in the global schema. Only by looking at data items may data elements become obvious. The example also highlights missing data in the local schema, and a possible amalgamated element in Band and Producer which together could correspond to Artist.

Identifying these semantic correspondences is almost entirely a manual task, sometimes even requiring domain experts to perform the matching. New research is attempting to automate this (Saleem *et al.*, 2008)) Since the next step, data integration, is fundamentally built on these mappings it is particularly important that this step is expertly completed.

2.5.3.2 Data Transformation

The semantic mappings from the previous step are used to write the relevant code (SQL) to transform and transfer the data into the global schema. Given the examples in Figure 2.10, if

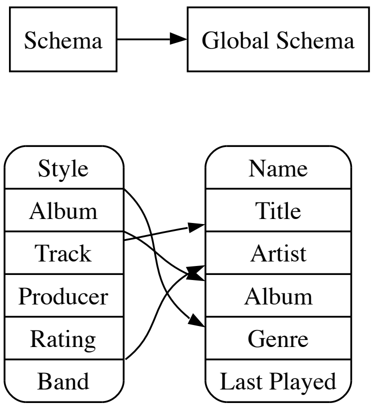


Figure 2.10: Schema Matching for transformation into the Global Schema.

both the source schema and global schema were in relational form, this stage would require an SQL query to transform the data (see Figure 2.11).

```
INSERT INTO into global_schema (Title, Artist, Album, Genre)
VALUES
(SELECT schema.Track,
Concat(schema.Band,| |, schema.Producer)AS Artist,
schema.Album, schema.Style
FROM schema)
```

Figure 2.11: SQL `INSERT` statement maps attributes from the (source) Schema into Global Schema attributes. The attributes *Band* and *Producer* are concatenated into the global schema attribute *Artist*.

This data merging step has three design considerations: performance, duplicate removal and data quality assessment. These issues can require considerable analysis and design effort.

In most cases, the above two steps are performed incrementally, i.e. the data are added into the global schema incrementally. The addition of the first data source is straightforward, the addition of the second and subsequent data sources, are more complicated, as the data need to be examined to remove duplicates. Data quality is considered after this stage, it is only once the data are brought together that the complexity of the data and the number of source data quality problems become evident. The physical transformation of data should homogenise and cleanse the data of inconsistencies across the data sources, making inconsistencies easier to spot.

Transformation steps are often performed with materialised views (or simply views). Views are a stored SQL query, which in this case compares the data in the global schema to the data that is in the local schema. Duplicates can be avoided either by including a clause in the view so that they are not included or they can be allowed in the view (as is sometimes required) and picked up by unique constraints on the global schema. These views also serve to speed up some of the data transformation process. The views also provide the first comparisons between different data sources and are therefore also used to analyse data quality and pick up data inconsistencies such as missing values or inconsistent use of attribute values. These processes are typically known as data scrubbing or data staging.

2.5.4 Data Warehouses - Update and Maintenance

The development of a data warehouse requires a considerable investment in time and resources. One point that needs to be addressed once the system is operational is maintenance and data refreshment. Most database systems require maintenance, such as for example, queries that need to be optimised and the addition or update of data or indexes. Similar maintenance requirements in a warehouse have the overhead of scale as warehouses, by definition, are larger than most of the data source systems, and as such the maintenance overhead is greater in terms of index sizes and backups.

The requirements of data refreshment should be considered at the early stages of development, and the rate of refreshment will depend on the purpose of the warehouse. All database systems have similar considerations however, due to the increased scale of data warehouses, performance during a data refresh can have a serious impact on users. In most cases maintenance and refreshment has to be done off-line. In some scenarios the data warehouses are not refreshed at all but retired and replaced with a system containing the new data.

Materialised views[1] and database triggers[2] are often used to maintain and refresh data. In these cases data refreshment can be either source driven (using views) or warehouse driven (using triggers). In a source driven architecture, when the source schemata are updated, the views simultaneously update the warehouse with the relevant changes. In a warehouse driven architecture, the warehouse is updated during specified down time, the new data are collected

[1]A Materialised view is the result of a SQL query where the result set is stored on disk.

[2]Database triggers are procedures that are stored in a database and are executed or "fired" when a table is modified.

into log tables and a trigger is fired once these tables reach a certain point (size or time driven). Clearly source driven refreshment has advantages, however, performance remains an issue and most databases can be refreshed more efficiently when they are taken off-line.

An alternative approach to data warehousing uses web services to facilitate cross-database queries. This mediated approach has also been successfully deployed for taxonomy (Page, 2005). In this system a user's query is captured by a mediating script (wrapper), which translates the query to the various data sources and returns the results to the user. The major advantage is that users have access to the most up-to-date data. Each source is mapped and the query mechanism is coded into a wrapper so that the user accesses each source through a uniform query interface. What can be delivered though are only those queries supported by each individual system. The warehouse approach has this additional advantage; the flexibility of data manipulation during transfer, and the ability to effectively query combined data as a unit. The warehouse approach is also more commonly used when data mining and cleaning are a necessary part of data integration.

2.5.5 Warehousing Taxonomic Data

As more and more taxonomic data becomes available to the wider user community, focus is beginning to shift towards understanding the distribution and quality of taxonomic data (Chavan *et al.*, 2005; Embury *et al.*, 2001). Data accuracy, consistency and completeness are issues the taxonomic community are beginning to address (Chapman, 2005a,b). By reconciling taxonomic data, we can begin to understand the quality of the data currently available and deliver more information to our user communities.

There is considerable benefit in combining and merging these taxonomic data sources. Aside from providing a single point of entry to taxonomic data, integrated data sources enable us to determine and understand data quality. Taxonomic names combined from several data sources into a common structure can be compared and verified against each other to identify inaccurate, inconsistent and incomplete data. Uncovering these data quality metrics (Fox *et al.*, 1994; Wang *et al.*, 1995) gives users the ability to understand and therefore use their data better. It can also be used to identify data that require cleaning or complete taxonomic review.

Integrated Taxonomic Information System (ITIS, 2006), the Universal Biological Indexer and Organizer (uBio, 2006) and Species 2000 (Bisby & Smith, 2000) were each built for specific user communities. The Sp2000 project provides federated taxonomic data and performs exceptionally well for the purposes and scope for which it was built. The problem arises for users who wish to use the data beyond this scope, for example, Sp2000 does not support the ability to search the individual data sources from which data are collected hierarchically, because it does not store the classifications from each of the data sources. uBio provides, at the moment, possibly the best taxonomic name search facility. These queries can be automated and integrated into other systems (Page, 2005) through their web services interface. However, the data they provide can not be downloaded into other databases, for example, a phylogenetic database. ITIS, which also compiles data from other data sources, carefully curate each datum they acquire and provide users with a single conservative view of each name. It is however, biased in data scope. Similarly, the NCBI (Federhen et.al, 2005) taxonomy is another excellent data source but biased reflecting only those organisms for which nucleotide or amino acid sequence information is available. There are many more examples of databases, each developed to meet specific user requirements (Deprez *et al.*, 2004). As a result taxonomy now has an enormous web presence yet none of these taxonomic data sources meet the requirements of TreeBASE as outlined.

The number of online taxonomic resources has now made it easier to collate taxonomic information (Bisby *et al.*, 2002; Gewin, 2002). “Data Warehouse” technology enables data to be brought together, integrated and transformed into a common structure. This increases the accessibility of the data to wider audiences by remodelling the data for their specific requirements. Generally, the source systems are designed for experts in the field, leaving non-experts put off by the interfaces and the overwhelming quantity of data. In most cases this remodelling simplifies data, making it accessible to non expert users and used outside its’ original design scope. This thesis goes on to outline the development of a taxonomic data source for TreeBASE, the Taxonomy and Classification Database (TCl-Db). In the warehouse architecture of TCl-Db, data from several taxonomic data sources are replicated and maintained in a common structure, increasing data coverage and adding links across the data sets. The data in TCl-Db is also transformed to enable hierarchical queries.

2.6 Summary

This chapter gives an overview of the complexities of taxonomic data. Regular changes to biological taxonomy result in name changes, synonyms, homonyms and many classificatory opinions. As a result biological taxonomy cannot be used as an information retrieval system. It is particular difficult to use taxon names to retrieve data. Even though many taxonomic database exist and these problems are being addressed, currently, the taxonomic requirements of the systematics community are not well supported. TreeBASE does not contain an adequate taxonomic infrastructure that supports taxonomically intelligent queries for data retrieval. Given the large number of online taxonomic database and the benefits provided by data integration, a data warehouse approach to resolving the taxonomic deficiencies of TreeBASE forms an ideal solution.

The following chapter details the design and implementation of TCl-Db. Taxon names and classifications from several data sources are combined into one queriable structure that supports expansion of vernacular, synonym and higher taxa query terms.

Chapter 3

Database Design and Implementation

The previous Chapter detailed the requirements for a taxonomic infrastructure for TreeBASE. This Chapter outlines the database structure of TCl-Db, the database that was built to meet those requirements.

3.1 Introduction

The taxonomic requirements of TreeBASE, and particularly the need to support of information retrieval, prompted the development of TCl-Db, a data warehouse of taxonomic names and classifications. Currently, no taxonomic database meets the requirements of the systematics/tree building community with respect to data coverage of taxon names and classifications. TCl-Db facilitates broader access to taxonomic data, beyond its expert community, through an integrated view of taxonomic data. The database structure enables the types of queries the systematics community would expect to perform. These queries are: hierarchical queries (the use of higher taxa names as the search term with the full classification below that term returned in the result set); and queries such as synonyms and vernaculars that expand to related terms.

TCl-Db uses a data warehouse approach to perform taxonomic data integration. In a data warehouse, the data are gathered from multiple sources and collated into a single structure. This approach is particularly useful to the systematics community, since it not only addresses the issue of data scope, but is also scalable and highly configurable, allowing data to be restructured to enable specific requirements. These requirements are outlined in this chapter. The architecture of the TCl-Db data warehouse, the databases that contributed data, and the global schema structure developed to hold the integrated data are described.

3.2 Requirements

3.2.1 Data Retrieval

When querying a database system the results returned are those data that satisfy the given query. This is referred to as **data retrieval** and in relational database systems it is accomplished by the query language SQL. Given well defined structure and semantics, a well formed query will return exactly those data that satisfy that query. In **information retrieval**, ideally, a given query is understood by the system, there is an element of interpretation through related terms or categorised topics (Fast *et al.*, 2002). The query does not have to be exact and the data returned is not that which matches the query but that which is relevant to the query. For example, a search through the TreeBASE data using a query on the vernacular term “Song Sparrow” will return data that matches that term exactly. Such a query will not return data including associated terms i.e., the scientific name *Melospiza melodia.* The database structure and data content of TreeBASE will only return data for a query if that data exists. If, for example, the term “Song Sparrow” exists, data will be returned, however, the data attached to *Melospiza melodia* will not. Inherently, a biologist is really talking about *Melospiza melodia* when he uses the vernacular “Song Sparrow” therefore, these users would expect the query to include both terms. In most cases it is also expected that a hierarchical query, a query using a higher taxon name, would return not just the data associated with that string but all relevant data, including subordinates of that taxon. Hierarchical queries are commonly used in “drill down” searches through generalised terms and as such play a valuable role in information retrieval. Currently, TreeBASE performs only data retrieval. The database was built specifically to enable effective taxonomic queries through TreeBASE through query expansion.

Hierarchical Queries

The hierarchical structure of taxonomic data is instinctively recognisable. A biologist can recognise a taxon name simply by its structure or its name ending. This organisational structure was originally designed to enable biologists to commit the data to memory (Cain, 1959) and enable

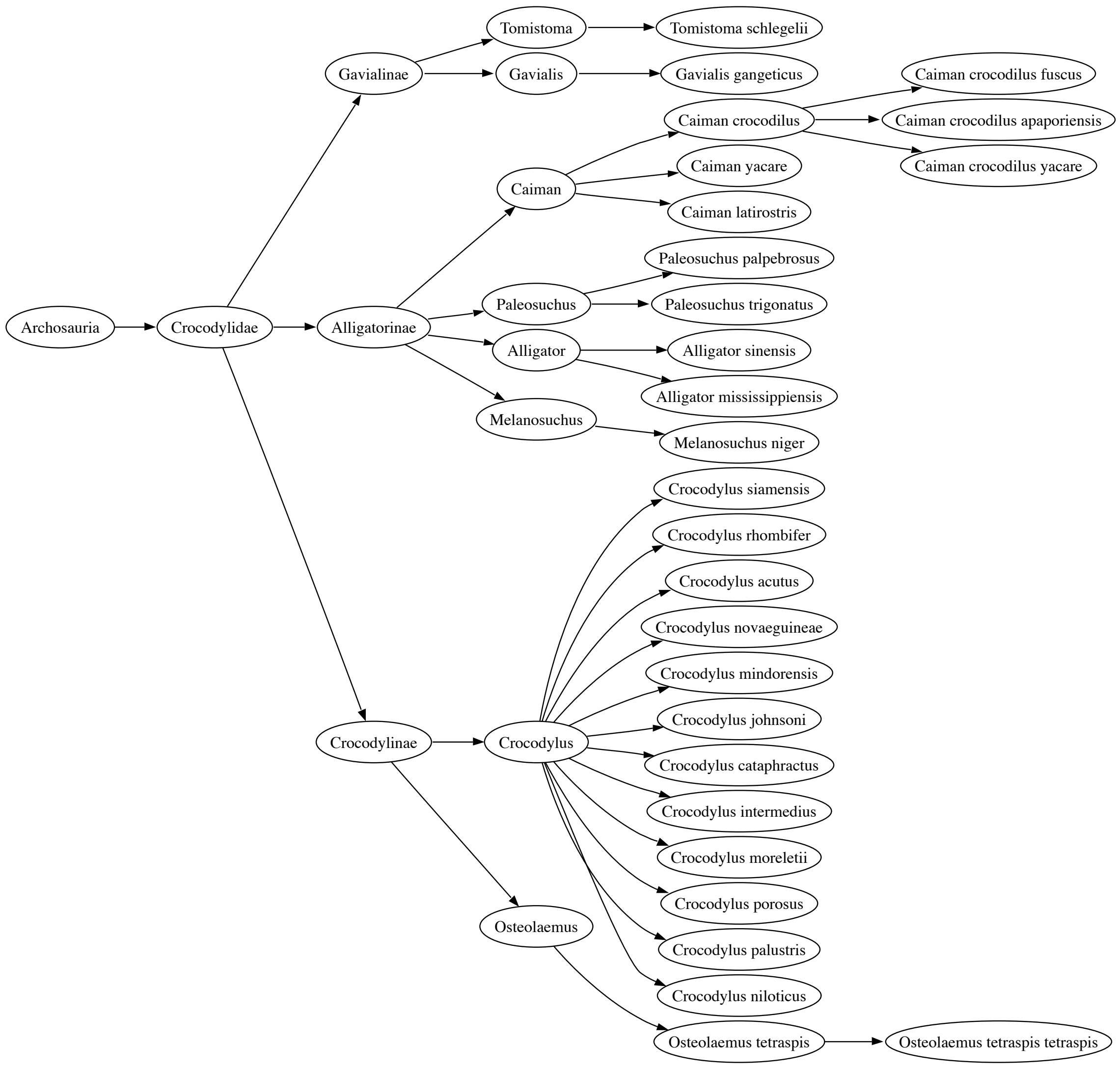


Figure 3.1: NCBI Classification of the family Crocodylidae.

them to identify and place newly discovered organisms into the system. For many biologists higher taxon names are a natural access point into databases such as TreeBASE. The results of a taxon name search should return that name in the context of its position in the classification and its usage in terms of validity or synonymy. In a database that is taxonomically aware, such as GenBank, hierarchical queries such as, "find all sequences for the genus *Crocodylus*" or "all sequences for the kingdom Fungi" are easy to specify. A hierarchical query enables a user to enter a broad search term and have the query expand through the hierarchy. This gives the user the opportunity to refine and adapt their search based on the result set. For example, a search on a taxonomic order should return all families, genera and species. Figure 3.1 shows an example of the results expected given the search term “Crocodylidae”. However, the differing classifications means hierarchical queries are not straightforward, since biologists may wish to use different classifications in these searches. Hierarchical queries on different data sources often return different result sets. Figure 3.2 A and 3.2 B are representations of the classification for the class Aves in NCBI (A) and ITIS (B). This circular representation of the hierarchy highlights the structural differences between the two classifications. When the two classifications are overlaid in Figure 3.2 C, with ITIS names in red and NCBI names in BLUE, we clearly

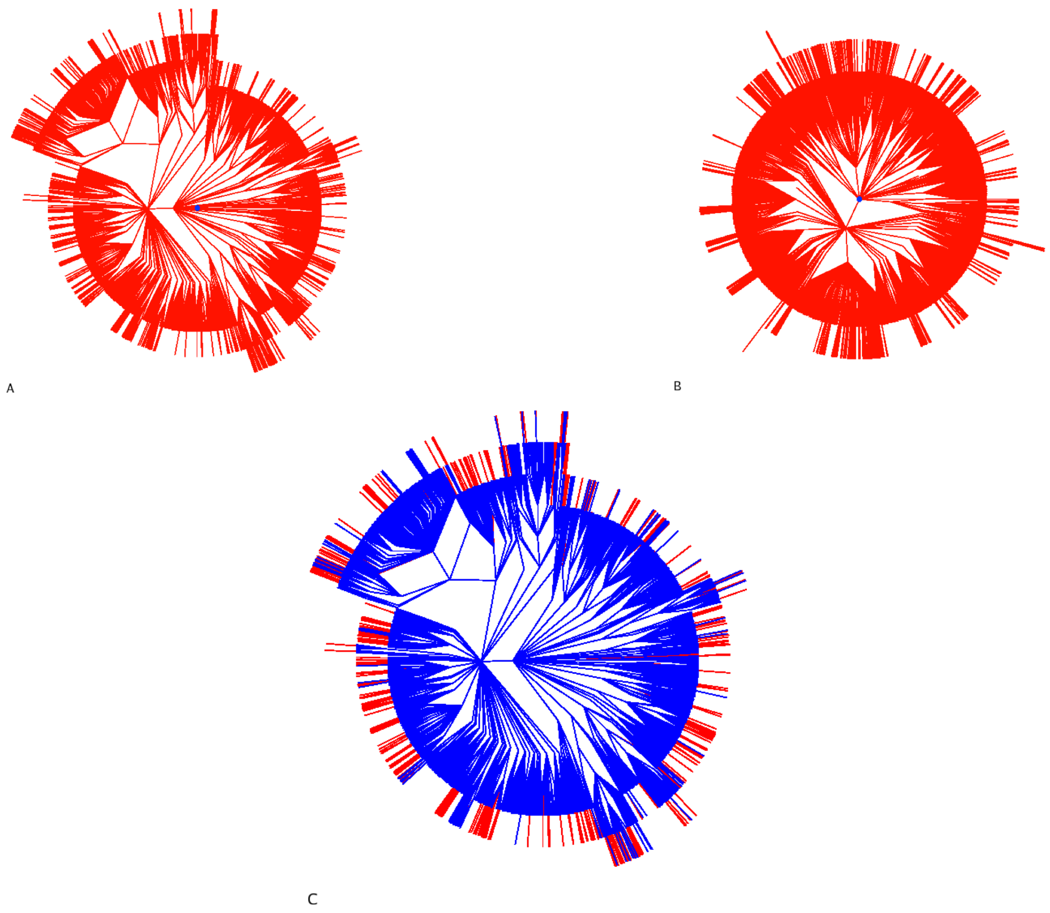


Figure 3.2: NCBI and ITIS Aves Trees. This figure highlights the difference in the classification of Aves in NCBI (A) and ITIS (B). C overlays names common to both ITIS and NCBI on to the NCBI classification.

see little overlap above the leaf nodes. Considering these different classification opinions it would be inappropriate to impose one classification on users. Therefore, a part of the design criteria of TCl-Db was to give users a choice of classification. This was also timely since most other taxonomic database amalgamations such as uBio and Sp2000 were focusing on gathering names and building global checklists rather than the classifications. uBio extended their remit to classifications.

Supporting Query Expansion for Synonyms and Vernaculars

The intertwining of names into the hierarchical structure has an adverse side effect when things change or are moved. The taxonomic system is in constant flux as new organisms are discovered and introduced into the hierarchy (Froese *et al.*, 1990), which often results in the movement of names in the hierarchy to accommodate additions and the subsequent changes to the names to fit into the new rank, as outlined in the previous chapter. Data additions that cause changes to the classification can be particularly severe since those changes have a rippling effect on the data below it. Where hierarchical data structures fail is in the lack of data management, as there is no mechanism to manage and share changes and additions to classifications provided by the expert (Froese *et al.*, 1990). As a result, data can be misused by users who continue to use those names they are aware of. For example, a user conducting a search with the term *Phoebastria albatrus* may not be aware that there are other names associated with that organism i.e., the synonym *Diomedea albatrus* and the vernacular “Short-tailed albatross” (Figure 3.3). Therefore, explicit in the user requirements is the ability to expand queries to include associated terms. Synonym and vernacular queries terms and their Latin names should be linked, so that queries can expand to include data associated with the linked terms. In a search interface a user may then enter either one of the above names as a search term, with the same result set returned.

Data coverage

The differences in classification between ITIS and NCBI have already been highlighted, however, these databases also differ significantly in data coverage, as shown in detail in Chapter 5. Particularly obvious differences are the coverage of data in bacteria and fungi where molecular data has played a much greater role in discovery and identification. In order to effectively use taxonomic data as search terms, the systematics community require an integrated global view of taxonomy that covers the breadth of available taxonomic data.

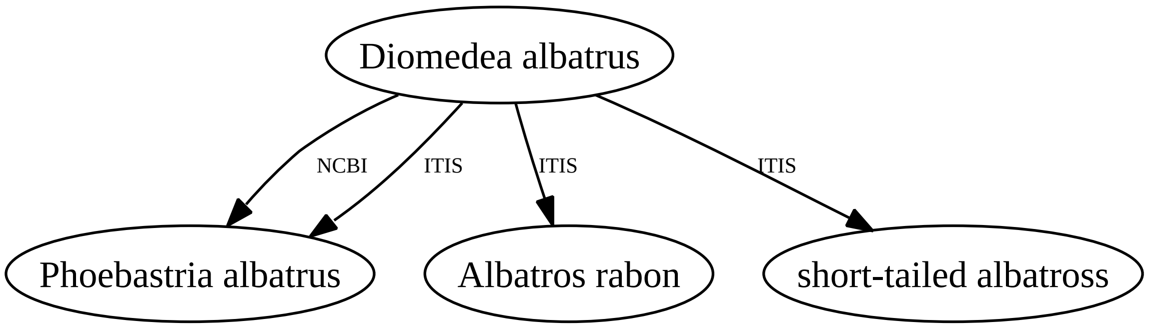


Figure 3.3: This figure shows linked names for one organism *Diomedea albatrus.* A search using any one of these terms will return all of the terms in the result set. The arrows show how the names are linked within the database. A simple search on the source databases using the term *Phoebastria albatrus* would not return "Short-tailed albatross" since there is no direct link between these terms.

Each of the requirements outlined above: data retrieval, query expansion and data coverage can be addressed through data integration.

3.3 Data Warehouse

The traditional method used to integrate and inter-operate between multiple data sources is to database using a warehouse approach. This approach involves migrating data from multiple sources into a common structure so that the data can be queried as a unit.

The warehousing approach to data integration is described in the previous chapter. It is well established and well supported in database technologies (Ullman *et al.*, 2001). An alternative approach to data warehousing uses web services to facilitate cross-database queries. This mediated approach has also been successfully deployed for taxonomy by Page (2005). In this system a user's query is captured by a mediating script (wrapper), which translates the query to the various data sources and returns the results to the user. The main advantage of this is that users have access to the most up-to-date data. Each source is mapped and their query mechanism is coded into a wrapper. The user accesses each data source through a uniform query interface. However, only those queries supported by each individual system can be delivered in the integrated wrapper. The specific requirements of enabling hierarchical, synonym and vernacular queries may not be available within each source. The warehouse approach does not have this disadvantage. In fact, it offers the flexibility of data manipulation during transfer, and the ability to effectively query combined data as a unit. The warehouse approach is also more commonly used when data mining and cleaning are a necessary part of data integration. The advantage from our perspective is that during data migration data can be restructured to enable specific user requirements. The disadvantage, however, is that this approach replicates data, as keeping data up-to-date adds a significant overhead to managing the system.

Given the requirements outlined above and specified in Section 2.4.3, data integration using a loose federated system would be insufficient. In loosely federated systems the data sources remain autonomous and maintain control over the structure of the data. Therefore, as a federation the data can not be transformed effectively to enable hierarchical queries. However, a materialised data warehouse copies data locally. This enables data re-modelling to support hierarchical queries and the ability to build new data structures to enable query expansion. Additional advantages offered through a materialised approach are reliability and scalability. This is of particular importance since this system is envisaged to apply to secondary databases such as TreeBASE. A materialised data warehouse approach was deemed most appropriate to meet the requirements laid out. This would be built using a RDBMS. We were faced with two choices of RDBMS: MySQL (MySQL, 2006), open source and distributed under the GPL License, and Oracle (Oracle, 2006) which requires a license but is free to academics for teaching and research. Since data can be ported across relational systems with relative ease, the decision was ultimately based on which system provided the best tools for development and which system would deal better with the requirement of hierarchical queries.

3.4 Modelling hierarchical data

A hierarchy is an organisational model in which the highest level of organisation consists of a single entity. An entity at a lower level of organisation is related to only one entity at the next higher level but can be related to more than one entity at the next lower level. Entities at all lower levels are related by extension to the single entity at the highest level of organisation. Biological taxonomy is a containment hierarchy in which a set at one level contains all the sets below it. For example, a family is a superset of all the genera and species contained in that family.

Relational databases in general do not handle hierarchical data very well, especially recursive queries through hierarchical data. Two solutions are Nested sets and Materialised paths (Celko,

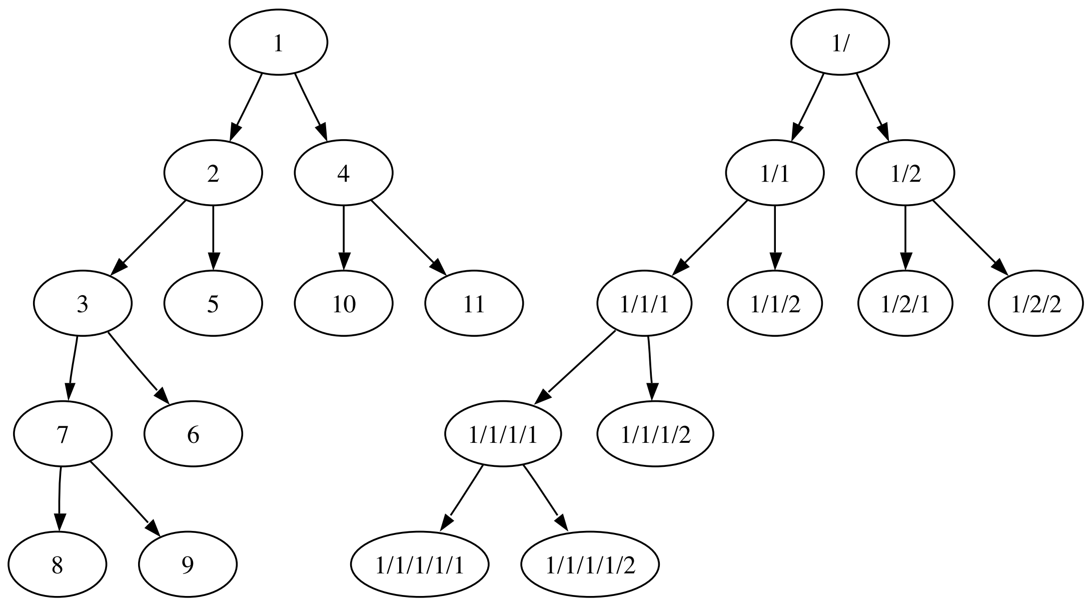


Figure 3.4: Hierarchical model represented as a node labelled graph on the left. The figure to the right represents the materialised path data for the same hierarchy.

2004; Tropashko, 2002). Also Oracle has a solution for recursive queries as an addition to SQL. These solutions are described below followed by a comparison that was performed to determine any performance advantages or disadvantages.

3.4.1 Materialized Paths

In this approach, the descriptive data for each node is the path from the root (the top) of the tree. A path is a string of characters that represents the edges connecting each node to the root node. Using the tree structure given in Figure 3.4, a hierarchy is represented on the left as node labelled graph and on the right the same hierarchy is shown with the nodes labelled with their materialised path string (similar to the directory path string in Unix).

3.4.2 Nested Sets

In Figure 3.5, the representation below the node labelled graph offers another representation that better reflects a containment hierarchy. Nested sets use this summativity representation. Each node in the tree is given a pair of numbered labels, to represent the inclusiveness of the node. The most inclusive pair is the root node and the least inclusive are the leaf nodes. For

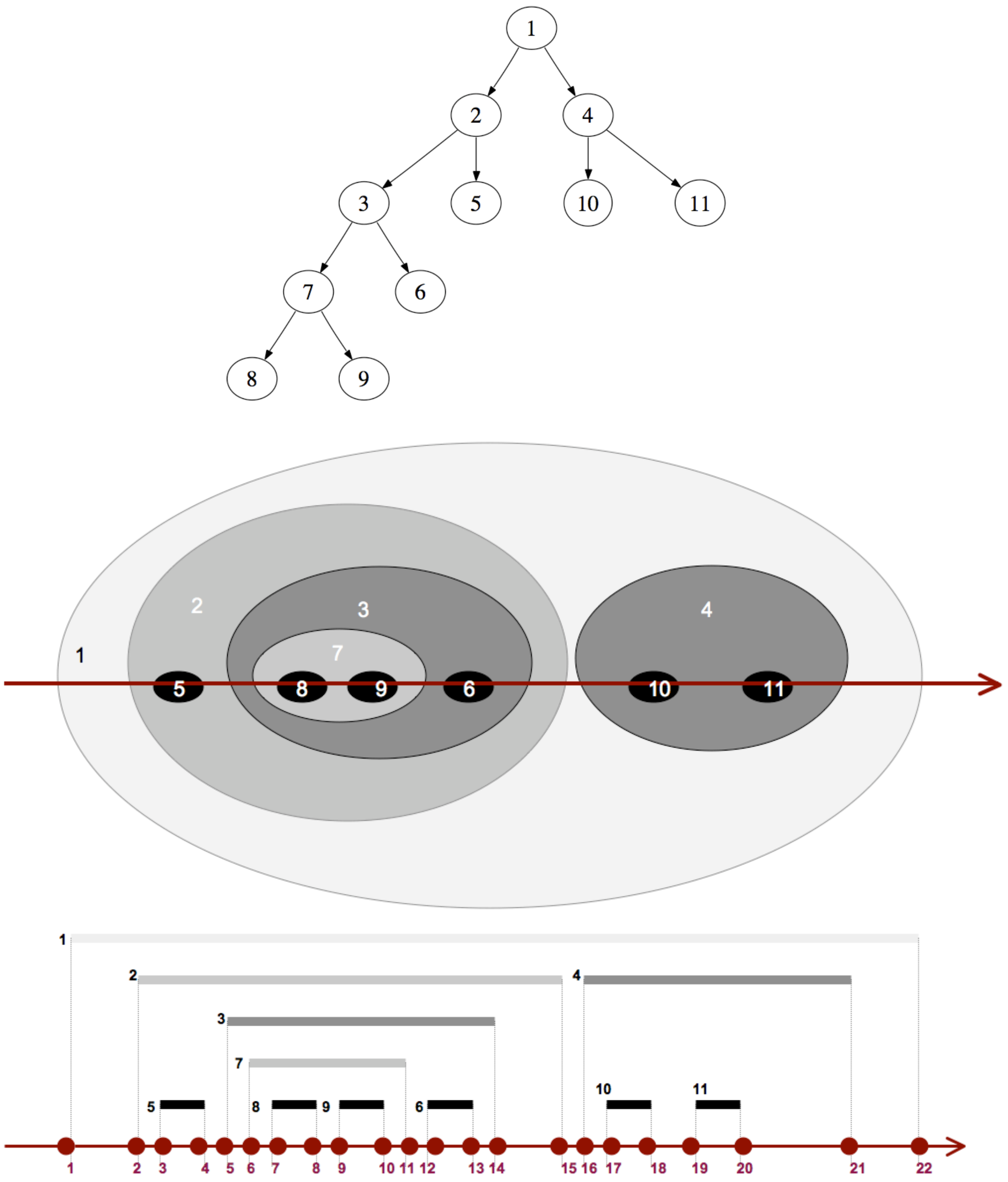


Figure 3.5: Summativity representation. This representation is created by collapsing each node into ovals and each oval into its parent ovals . Each oval represents a set containing nodes from the node labelled graph above. The nested sets are left and right numbers representing the containment. These are calculated by drawing a line through each oval, as the line comes through an oval a number is incremented and attached to the left (the beginning of the set) and then right (the end of the set) of each node.

example, the nested set for node 1 is defined by the labels 1 and 22, node 3 is defined by 5 and 14 and node 6, a leaf node, has the nested set 12 and 13. The nested set 12 and 13 for node 6 is contained in the set, 5 and 14, for node 3 which in turn is contained in the set 1 and 22 for node 1. These sets are calculated by drawing a horizontal axis through the the graph shown in the centre and at the bottom of Figure 3.5, each node is numbered as the axis passed through each boundary.

The nested sets and materialised paths offer an attractive solution because they are both database vendor free solutions. The advantage they offer is the ability to use these data in any RDBMS which makes the system portable. However, the disadvantage is that these data need to be calculated for each tree, thus adding a significant over-head to data update. This is particularly a problem if the tree structure changes or is updated as the paths and nested sets for the whole tree have to be recalculated. The Oracle CONNECT BY query does not have this added overhead since it uses only the parent-child relationship.

3.4.3 Performance Benchmarking

A benchmarking exercise was conducted on each form of hierarchical query to determine any performance advantage or disadvantage within Oracle and MySQL. Using the same table structures in Oracle 9i and MySQL 4 with the same indexes and constraints, the responsiveness of each database with each hierarchical query was tested.

The initial results show that both database implementations performed equally well in a small subset of the NCBI taxonomy tree, with Aves at the root of the tree (4645 rows in the table). We found, on this small dataset, that the differences in query response times were negligible, therefore the benchmarks were repeated on a larger dataset (the full NCBI Taxonomy tree with 162290 rows).

Using the larger data set, Oracle outperformed MySQL in both nested set and materialised path queries. In Oracle, the CONNECT BY query timed out and two sub queries (selecting a small branch of the tree) were also very slow to complete. The small difference between the nested sets and path queries is most likely due to the difference between Oracle and MySQL indexing. Nested sets are a numeric query (select all nodes between 1 and 22) while the paths are a textual query (select all nodes that match 1/*). Given the way SQL performs, we would expect the numerical, nested set queries, to have a performance advantage over the materialised path queries, however, the table below shows that the materialised paths significantly outperformed the nested sets for this data set. The results are summarised in Table 3.1.

Aves (4645 rows)		
Query	Oracle	MySQL

CONNECT BY
`select count(taxon_id)`
`from taxon start with taxon_name ='Aves'`
`connect by prior`
`taxon_id = parent_id`
	0.0	N/A

Nested Set
`select count(taxon_id)`
`from taxon`
`where left_id between 1 and 9290`
	0.0	0.01

Materialised Path
`select count(taxon_id)`
`from taxon`
`where path like '/%'`
	0.0	0.02

NCBI (162,290 rows)		
Query	Oracle	MySQL

CONNECT BY
`select count(taxon_id)`
`from taxon start with taxon_name ='Root'`
`connect by prior`
`taxon_id = parent_id`
	Timed Out	N/A

Nested Set
`select count(taxon_id)`
`from taxon`
`where left_id between 1 and 324574`
	0.0	0.45

Materialised Path
`select count(taxon_id)`
`from taxon`
`where path like '/%'`
	0.0	0.01

Table 3.1: Average benchmark times in seconds taken for each of the three hierarchical queries on Oracle and MySQL. Two data sets are used: the upper panel is the smaller Aves subtree of NCBI and the lower panel is the full NCBI tree.

Given the overhead of building the nested set and materialised path data, the sensible approach was to allow hierarchical data to be queried in more than one way. Oracle was ultimately the RDBMS of choice, as if the nested sets or paths could not be built, an alternative query, the CONNECT BY query, would still be available. Also, by giving a choice of mechanisms to perform hierarchical queries, the system would still be accessible and portable to other database products, including MySQL. The nested sets and materialised path data need to be calculated and an example of building this data in Perl is given in Mackey (2002). The program used here was written by Rod Page in C++ and performed very efficiently and calculated both nested sets and path strings with no additional cost in time. Since both data sets were created, both were included in the TCl-Db model.

3.5 TCl-Db Structure

The database design was based on the data model given below in Figure 3.6. This was transformed into the physical structure shown in Figure 3.7.

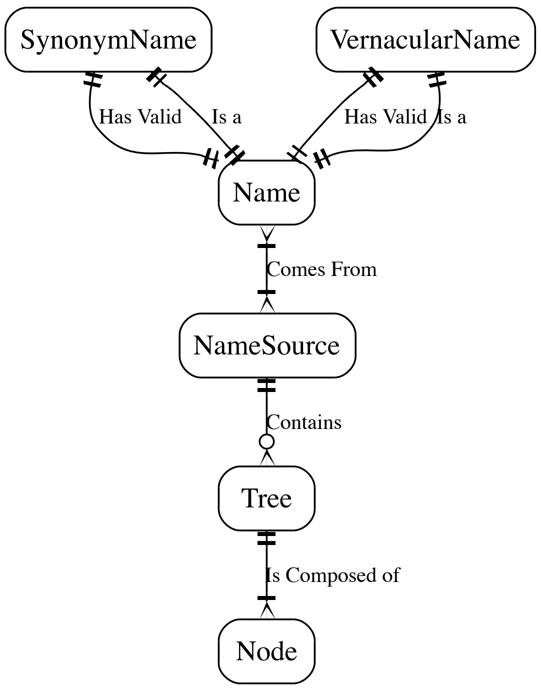


Figure 3.6: ER diagram representing the TCl-Db data model.

The entity NAME identifies a taxonomic name. The NAME entity has the following attributes: name_id, which uniquely identifies any given entity occurrence; name_text, which is the name; and name_usage i.e., valid, synonym or vernacular. NID is a globally unique identifier attached to the name upon entering the database. A name comes from one or more name sources and the NAME_SOURCE entity identifies the database from which a NAME originated. NAME_SOURCE has the attributes: source_id, source_db_name, ora_schema_name and URL. From the model in Figure 3.6, a name must come from one or more name sources, giving NAME and NAME_SOURCE a many to many (M:M) relationship. M:M relationships cannot be represented as simple attributes in either relation. To resolve this, the relationship is replaced with an association entity called ASSERTION (Figure 3.8), also used by Pyle (2004) and Berendsohn (1995). An ASSERTION is an instance of a taxonomic name in a name source. ASSERTION, as an association entity would normally be a key only, however, in TCl-Db this is where the source ids are stored as dbsource_id. The dbsource_id in ASSERTION represents the unique identifier of the name in the data source of origin (TSN in ITIS, taxonid in NCBI etc). Kingdom and rank are also placed in ASSERTION as discussed in more detail below.

The TREE entity identifies the trees that have been built from a particular NAME_SOURCE. Several different tree topologies can be built from one name source, for example, different classification opinions of the NCBI classification tree and edited versions of the ITIS classification tree. Several topologies of a name source's classification can therefore be loaded into the schema and traversed. A TREE entity identifies each topology and has the attributes tree_id, tree_name, description and source_id to link back to the source from which the classification was built. Each TREE must have one or more nodes describing the topology of the tree. Each TREE is composed of NODES (Figure 3.6). A NODE identifies the location of a NAME/ASSERTION in a particular classification TREE from a particular NAME_SOURCE. ASSERTIONS and NAMES are tied to each NODE via foreign keys. The attributes name_id and parent_name_id describes the parent-child relationship of each NODE, there is a check constraint on these attributes to make sure that the name_id and parent_name_id exist in NAMES. The parent_name_id and name_id together with

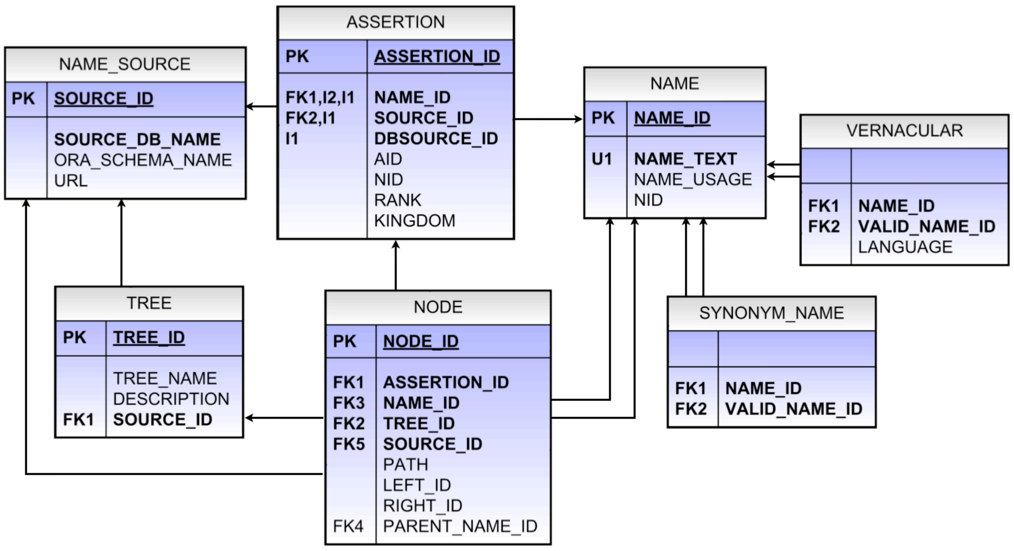


Figure 3.7: The TCl-Db physical data model. The divided boxes represent relations (tables), the name of the table is shown in the grey division and the columns and keys are given in the blue division. Constraints are labelled: Foreign Keys (FK), Primary Keys (PK), Unique (U), Not Null (I).

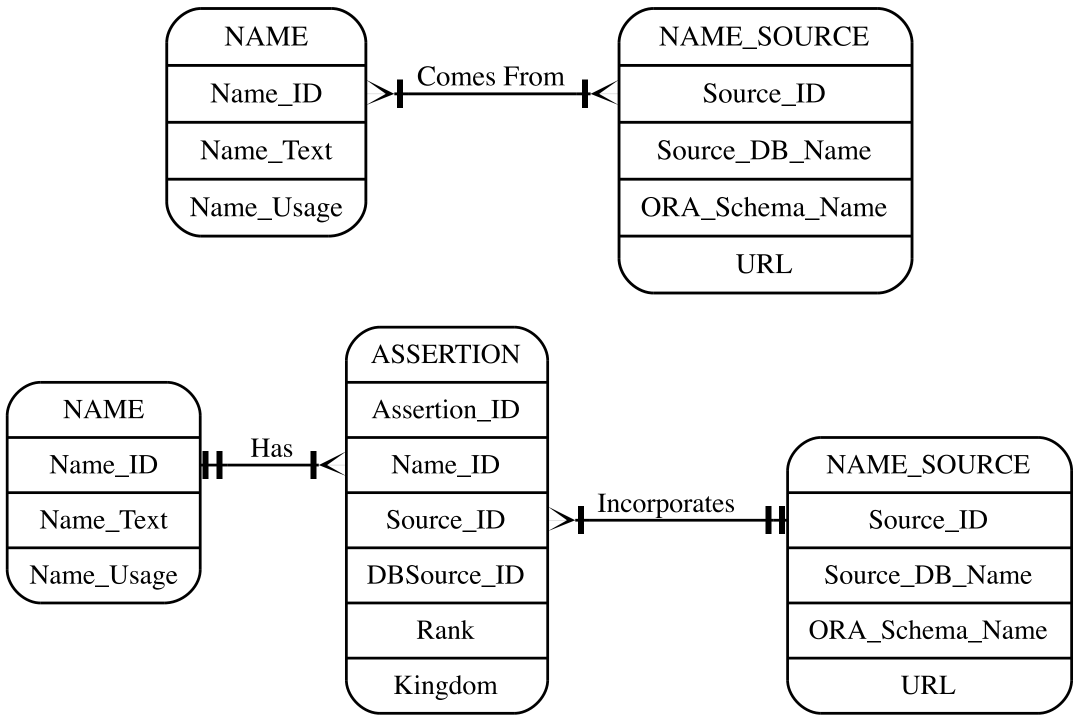


Figure 3.8: The many to many relationship between NAME and NAME_SOURCE (above) is resolved below with the association entity ASSERTION.

tree_id, are used in Oracle CONNECT BY queries. The location of each NODE in each classification TREE is also described by the attributes left_id, right_id for the nested sets representation and the attribute path stores for the materialised paths representation. (Celko & McDonald, 1995), (Celko, 2004).

Stable unique identifiers are attached to ASSERTIONS and to NAMES to enable other databases to link to TCl-Db. These are tracked using the AIDS_MV materialised view, for ASSERTIONS and NIDS_MV materialised view for NAMES. On entering the database, each name is given this unique and anonymous number. This identifier is guaranteed not to change on update. After a data load the following steps are employed to ensure stability in the identifiers. Firstly, the names are checked against the NIDS_MV view to get the NID if it exists. Secondly, if the name does not exist, a new NID is assigned and if the name does exist, the NID is updated from the view data. Finally, on completion of the update, the view is refreshed with the DBMS_MVIEW.REFRESH procedure. The same method is used for AID's on assertions.

The materialised views in the databases are refreshed on demand since many are ineligible for automatic refresh (i.e., on commit). These views are formed by complex queries, or, in the case of NIDS_MV and AIDS_MV, make reference to the non repeating expression SYSDATE. Mostly, the views are used to simplify and speed up data loads, so refreshment is performed during the data loads. These views actually serve to simplify data loading procedures, since the original queries to build the views are effectively stored in the schema and refreshed using just one simple procedure call. Thus, the views provide simplicity and increase the performance of the data load, and their maintenance forms part of the data load procedures.

3.5.1 Modelling rank and kingdom

With the exception of the attributes rank and kingdom, the entity ASSERTION is key only. There were several design options for these data, reflecting the complex relationship between NAME, NODE and ASSERTION. The relationships are shown in Figure 3.9.

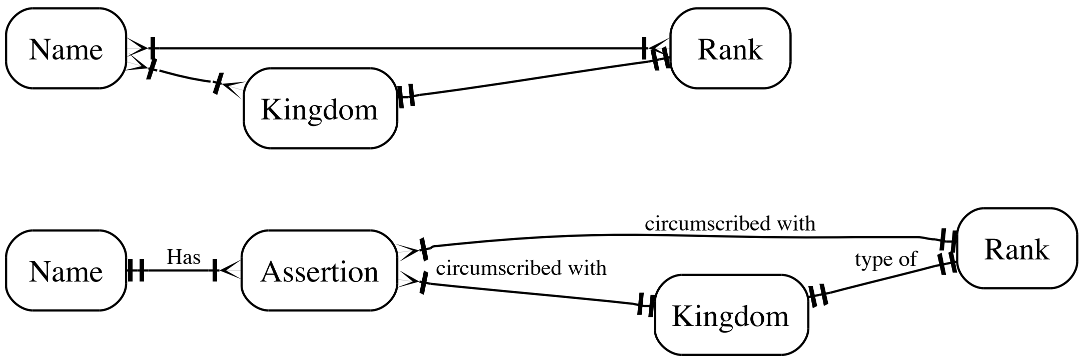


Figure 3.9: The many to many relationship between NAME , KINGDOM and RANK is resolved with association entity ASSERTION.

Ranks and kingdoms are attributes of a name, however, because the attributes of names can be different in each name_source, they are modelled as attributes of ASSERTIONS. This placement results in repeating values in ASSERTIONS. However, kingdom and rank have a restricted number of values. Kingdom can be only one of 5 values, and Rank, depending on the classification, also has a limited number of values, so that the repeating values are easily managed through check constraints during data load. Adding these as separate entities would have added complexity to the data model and data load process. In the pursuit of a simple model these were modelled as attributes of ASSERTIONS.

3.5.2 Modelling synonyms and vernaculars

SYNONYM_NAME and VERNACULAR are weak entities reliant on the foreign keys referencing the NAME entity. A NAME may exist without a SYNONYM_NAME ; a SYNONYM_NAME , however, can not exist without a NAME because both attributes of SYNONYM_NAME and VERNACULAR are foreign keys. These could have been modelled as a "usage" attribute, describing the usage of the name. In situations where different data sources treat the same name differently, this model would result in multiple values of usage per name. To avoid multi-valued attributes and self referencing on NAME, the weak entities SYNONYM_NAME and VERNACULAR are used instead.

3.5.3 Trees and Nodes

The classification trees for each NAME_SOURCE are modelled to enable hierarchical queries. Parent-child relationships through name_id and parent_name_id are used by the Oracle CONNECT BY query. The left_id and right_id are used in the nested set queries, and path is used by the materialised path query.

A NODE has two foreign keys. Source_id references NAME_SOURCE and tree_id references TREE. The source_id constraint is not actually necessary since the foreign key to assertion_id referencing ASSERTION accomplishes the same thing: a NODE is linked to its NAME_SOURCE through the assertion_id. For example, the query in Figure 3.10 returns the number of names below Aves (name_id 13232598) using its assertion_id 11951770 which links it to the name_source ITIS. This compares to the query shown in Figure 3.11 which uses the foreign key tree_id. When using tree_id, the join to the assertion table is not required. The query is much faster because it does not have to compute a join, as the data is accessed from only one table. Also, more than one classification can be stored for a NAME_SOURCE, as for some name_sources using assertion_id would return data from more than one tree. Therefore the first query using assertion_id only works when there is only one TREE for a NAME_SOURCE. The addition of extra foreign keys speeds up a number of queries that are used in the application described in Chapter 5. The foreign keys were therefore included, in order to simplify and speed up hierarchical queries.

Hierarchical queries using materialised paths

Example nested set queries are shown in Figure 3.10 and Figure 3.11 The nested set and path data have been included to make the system more accessible and portable to other database products, including MySQL. The nested set mechanism is described by Celko (2004), and

```
SELECT count(a.name_id)
FROM node a, assertion b
WHERE a.assertion_id = b.assertion_id
AND a.left_id BETWEEN
(SELECT left_id FROM node
WHERE name_id = 13232598 AND assertion_id = 11951770 )
AND (SELECT right_id FROM node
WHERE name_id = 13232598 AND assertion_id = 11951770 )
```

Figure 3.10: SQL query using nested sets. This query used assertion_id to traverse the classification from Aves in ITIS.

```
SELECT count(name_id)
FROM node
WHERE tree_id =1
AND left_id BETWEEN
(SELECT left_id FROM node WHERE name_id = 13232598 AND tree_id = 1 )
AND
(SELECT right_id FROM node WHERE name_id = 13232598 AND tree_id = 1 )
```

Figure 3.11: SQL query using nested sets. This query used tree_id and name_id to traverse the classification from Aves (name_id 13232598) in ITIS (tree_id 1).

these data, currently, need to be calculated using graph algorithms. An example query using materialised paths is shown in Figure 3.12, these hierarchical queries are described in detail in the following chapter.

Hierarchical queries using Oracle's CONNECT BY statement

The CONNECT BY query is an extension to SQL that was implemented by Oracle specifically to enable hierarchical queries using parent-child relationships. Within TCl-Db the CONNECT BY query uses the parent-child relationship modelled by the attributes name_id and parent_name_id in the NODE entity. An example, for the name_id (e.g., 13232589 for the genus *Crocodylus*) is shown in Figure 3.13. Further examples are given in the following chapter.

Example materialised path query
SELECT path
FROM node
WHERE tree_id = 1
AND name_id = 13232589
SELECT count(*)
FROM node
WHERE tree_id = 1
AND path LIKE
/1/30/3/4/4/1/1%

Figure 3.12: SQL query using materialised paths. This query used tree_id and name_id to traverse the classification from Aves (name_id 13232598) in ITIS (tree_id 1).

Example CONNECT BY query
SELECT node_id
FROM node
WHERE source_id = 116
AND tree_id = 1
START WITH (name_id = 13285208 AND tree_id = 1)
CONNECT BY PRIOR parent_name_id = name_id

Figure 3.13: SQL query using CONNECT BY. This query used tree_id and name_id to traverse the classification from Aves (name_id 13232598) in ITIS (tree_id 1).

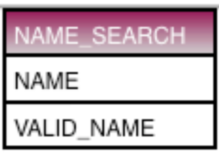
3.6 Application Tables and Query performance

The schema has not been de-normalised and the physical structure conforms very closely to the original conceptual structure. The requirement to ensure good performance of data loads kept the warehouse structure as simple as possible. Query considerations did go into the design, for example, by modelling the NODE and TREE data as described above. However, query performance did not drive the data warehouse design. Query performance was addressed, instead, through the use of a de-normalised structure overlaying the warehouse structure. These tables and materialized views are built specifically to guarantee good performance in application queries.

The NAME_SEARCH table (Figure 3.14) is an amalgamated table of data from NAME, SYN-

ONYM_NAME and VERNACULAR. It also contains all identified homonyms.

```
INSERT INTO name_search
SELECT get_name_text(name_id) AS name,
get_name_text(name_id) AS valid_name
FROM name
WHERE name_usage = 'valid';
```



```
INSERT INTO name_search
SELECT get_name_text(name_id) AS name,
get_name_text(valid_name_id) AS valid_name
FROM synonym_name;
```

```
INSERT INTO name_search
SELECT get_name_text(name_id) AS name,
get_name_text(valid_name_id) AS valid_name
FROM vernacular;
```

```
INSERT INTO name_search
SELECT a.name_text, a.name_text||'('||b.kingdom||')' AS valid_name
FROM NAME_KINGDOM_DUPS a, assertion b
WHERE a.name_id = b.name_id
AND a.name_usage = 'valid'
AND b.kingdom is NOT NULL
GROUP BY a.name_text, b.kingdom;
```

Figure 3.14: Insert statements used to load the application table NAME_SEARCH

The queries in Figure 3.14 use a function, GET_NAME_TEXT. A number of functions were created to increase query performance (Figure 3.15). They were built for common data items, such as name_text and in most cases are used to simplify queries by reducing the number of table joins.

get_name_text	SELECT get_name_text(parent_name_id) FROM node WHERE name_id = 13232598
get_source_name	SELECT get_source_name(source_id) FROM node WHERE name_id = 13232598
get_itis_path_name	SELECT get_itis_path_string(name_id) FROM name WHERE name_text = 'Aves'
get_ncbi_path_name	SELECT get_ncbi_path_string(name_id) FROM name WHERE name_text = 'Aves'

Figure 3.15: SQL examples using functions, GET_NAME_TEXT, GET_SOURCE_NAME, GET_ITIS_PATH_NAME and GET_NCBI_PATH_NAME.

The hierarchical queries proved to be particularly slow. Even the two functions GET_NCBI_PATH_NAME and GET_ITIS_PATH_NAME were not fast enough, and therefore, tables were created to store pre-computed path strings for particular groups within ITIS and NCBI data source classifications. For the Aves group two tables were created, for example, these are ITIS_AVES_PATH_STRINGS, NCBI_AVES_PATH_STRINGS.

3.7 Procedures and Views

In addition to the entities and relationships described, the database also contains PL/SQL procedures and materialized views. The PL/SQL procedures move data from each data source schema into the TCl-Db schema. The database contains a schema for each source database including: NCBI (Federhen et.al, 2005), ITIS (ITIS, 2006), SP2K (Bisby & Smith, 2000), GRIN (USDA, 2000), MSW (Wilson & Reeder, 1993) and other checklists. Once these source database schemas are built, the data are loaded using Oracle's SQLLDR utility. The PL/SQL procedures then move the relevant data into the TCl-Db schema. Materialised views are used by these procedures to help speed up the data transfer across the schemas. A materialized view is a snapshot of data from a query performed on master tables. In this case, tables in the source database schemas. By pre-calculating expensive joins and aggregations into a materialized view, performance of the data transfer is significantly improved. For example, the materialized views SP2K_NAMEIDS_MV calculates the names that are already in TCl-Db NAME table and stores the NAME_ID and DB_SOURCEID, so that the addition of these known names to the ASSERTION table during data load is accomplished by querying one table. The procedures used for data load are detailed in the following chapter.

3.8 Summary

This chapter describes the architecture and schema design of TCl-Db. The database stores not only the taxonomic names but also the full classifications for each data source. This gives users access to differing classification opinions in one data structure. The supported hierarchical queries are outlined with SQL examples. Application tables that were built, for example, to enable the use of linked names in searches through the NAME_SEARCH table, and functions that are used to improve query performance are also described. The next chapter details the procedure used for populating the data warehouse and data sources that were merged into the TCl-Db structure.

Chapter 4

Populating the Database

This Chapter describes in detail the procedures followed during database loading. This is done for each of the data sources in the following order: ITIS, NCBI, GRIN, Sp2000, Mammal Species of the World and finally other smaller resources.

4.1 Introduction

In this chapter we present each of the data sources and the protocol used for loading the data. For each of the data sources this can be described in 3 steps, (1) assembling local version of the source database, (2) mapping source schema elements to TCl-Db and (3) loading data into the TCl-Db schema.

The application architecture is depicted in Figure 4.1. The data sources used within TCl-Db were all downloaded and replicated into an Oracle database as separate silos (schemas). In most cases, the data sources were replicated into their silos in their native format. We created the table structures that represented the structure of the source files. Since the data were not manipulated into another format, there was no possibility of compromising the integrity of the data with an additional transformation step. The TCl-Db warehouse was then populated with data from several data sources. These are given in the order in which they were loaded. A full list of contributing data sources is shown in Table 4.1.

The following section gives background information for each of the data sources and a description of the schema mapping and data load process.

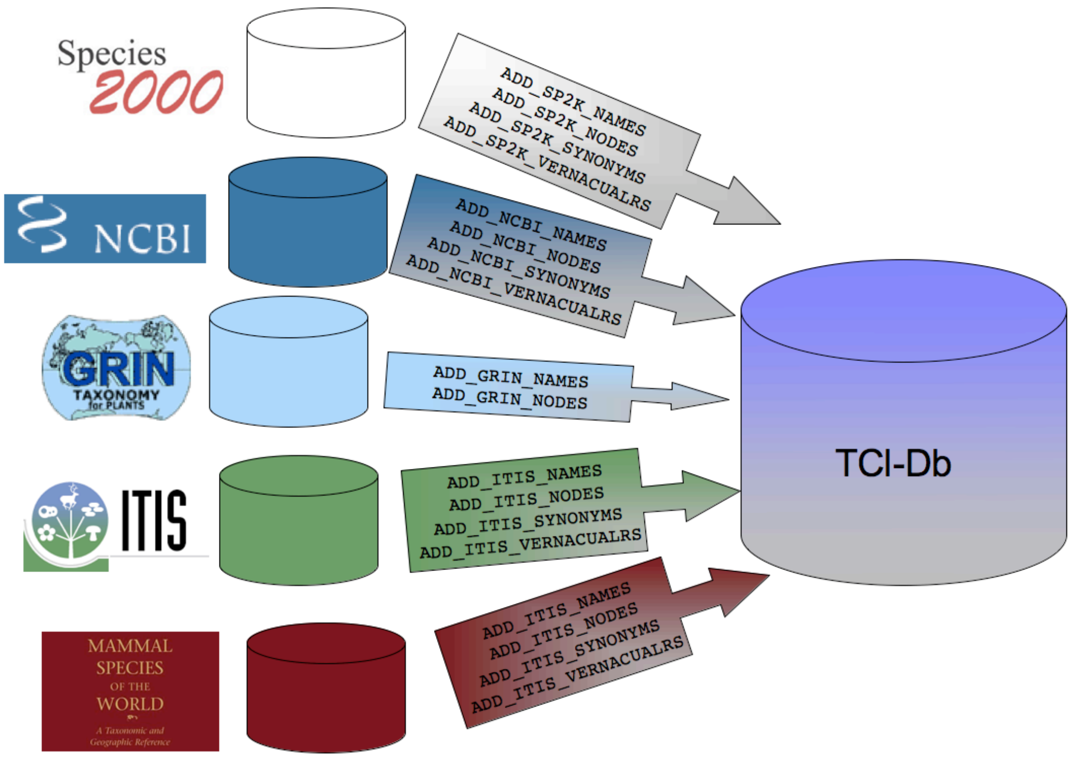


Figure 4.1: The database architecture. The diagram shows the five larger data sources within the database. These are: NCBI (National Center for Biotechnology Information), ITIS (Integrated Taxonomic Information System), MSOW (Mammal Species of the World), GRIN (Germplasm Resources Information Network), and Species 2000. Other smaller checklists have also been added. The PL/SQL procedures for moving data between the schemas are stored within TCl-Db.

Data Source	Download Date/Version	Name count
ITIS	January 2004	413227
ITIS	October 2005	78847
GRIN	July 2005	94146
NCBI	September 2004	273404
NCBI	October 2005	346840
SP2K	2006 Annual Checklist	1262469
ALGAEBASE	July 2005	38150
MSOW	July 2005	6058
nam980612		12034
American Ornithological Union	AOU (1983)	4936
American Ornithological Union	AOU (1998)	2755
Sibley and Monroe	Monroe & Sibley (1997)	11932
Peters	Peters (1987)	11267
Clements	Clements (2000)	19305
Bird_names	IOC World bird names 2006	19313
Morony, Bock, and Farrand	J.J. Morony *et al.* (1975)	11455

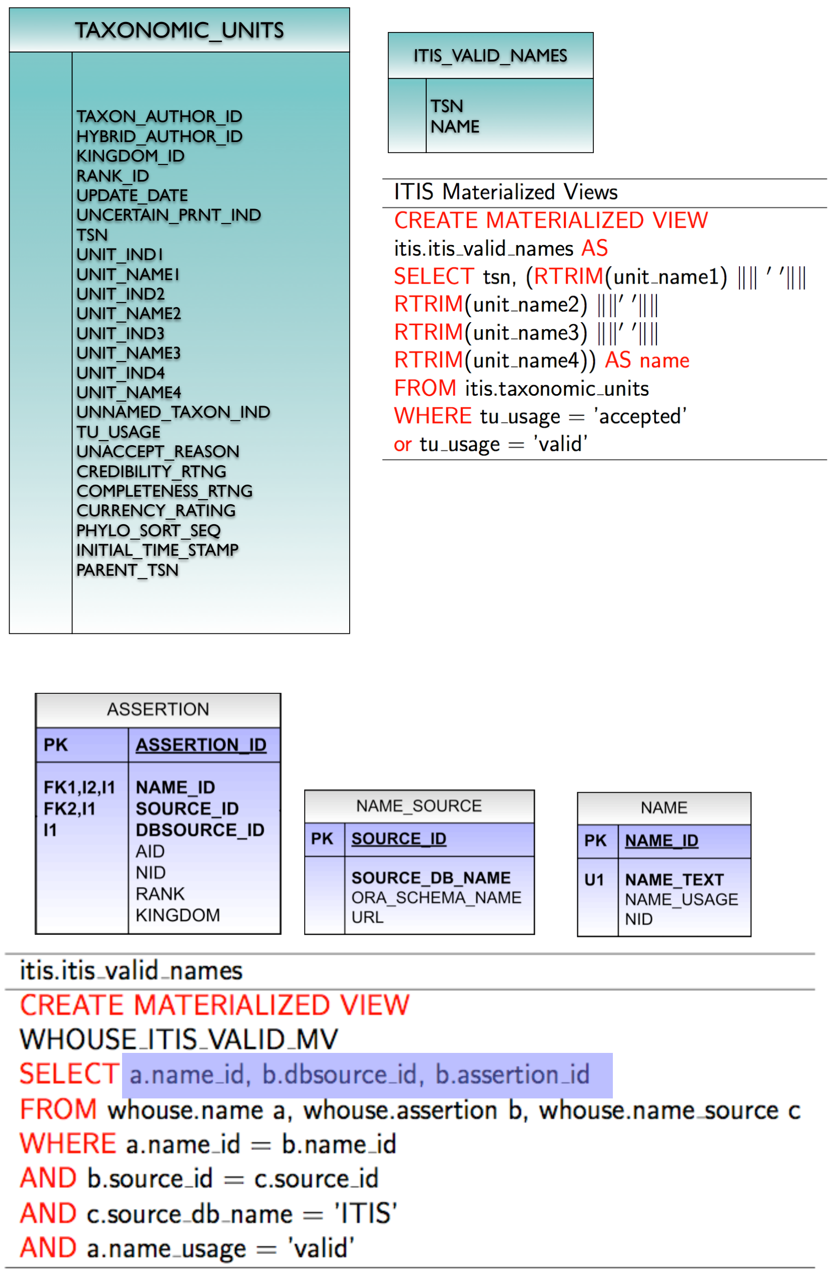
Table 4.1: Summary of data sources.

4.2 ITIS

The Integrated Taxonomic Information System (ITIS) (ITIS, 2006) is a partnership of federal agencies and organisations from the United States, Canada, and Mexico. It is primarily a taxonomic database serving data for " biota of interest to North America", though the data are curated by experts from around the world and the taxa are not limited to those native to North America. The taxonomic scope includes: the ITIS classification and scientific names and common names in English, French, Spanish, and Portuguese. The data are available for download in relational form. The downloaded files include an SQL script for building the table structures and a separate dump file for each table. This script was manually edited to remove the source RDBMS specific structures so that it could be used within both MySQL and Oracle RDBMS. After copying the source schema into TCl-Db, the data were loaded using Oracle's SQLLDR utility.

4.2.1 Schema mapping and Integration

ITIS was the first data set loaded. The original database dump contained an SQL script which, after some modification, was used to replicate the ITIS dump into a data silo within our Oracle instance. The transformation of ITIS data into TCl-Db's global schema uses four PL/SQL procedures: ADD_ITIS_NAMES, ADD_ITIS_NODES, ADD_ITIS_SYNONYMS and ADD_ITIS_VERNACULARS. In addition to the ITIS tables, there are two materialized views used in the load procedure



ITIS Materialized Views

```
CREATE MATERIALIZED VIEW
itis.itis_valid_names AS
SELECT tsn, (RTRIM(unit_name1) ||| ' '|||
RTRIM(unit_name2) |||' '|||
RTRIM(unit_name3) |||' '|||
RTRIM(unit_name4)) AS name
FROM itis.taxonomic_units
WHERE tu_usage = 'accepted'
or tu_usage = 'valid'
```

itis.itis_valid_names

```
CREATE MATERIALIZED VIEW
WHOUSE_ITIS_VALID_MV
SELECT a.name_id, b.dbsource_id, b.assertion_id
FROM whouse.name a, whouse.assertion b, whouse.name_source c
WHERE a.name_id = b.name_id
AND b.source_id = c.source_id
AND c.source_db_name = 'ITIS'
AND a.name_usage = 'valid'
```

Figure 4.2: Definitions of the materialized views, ITIS_VALID_NAMES and WHOUSE_ITIS_VALID_MV

ITIS_VALID_NAMES and WHOUSE_ITIS_VALID_MV whose definitions are given in Figure 4.2. The first view created is ITIS_VALID_NAMES. It concatenates the taxonomic unit attributes in the ITIS table TAXONOMIC_UNITS into a single attribute called NAME, for valid and accepted names. This view is then used in the procedure ADD_ITIS_NAMES (Figure 4.3). The relations NAME, ASSERTION and NAME_SOURCE are populated by this procedure.

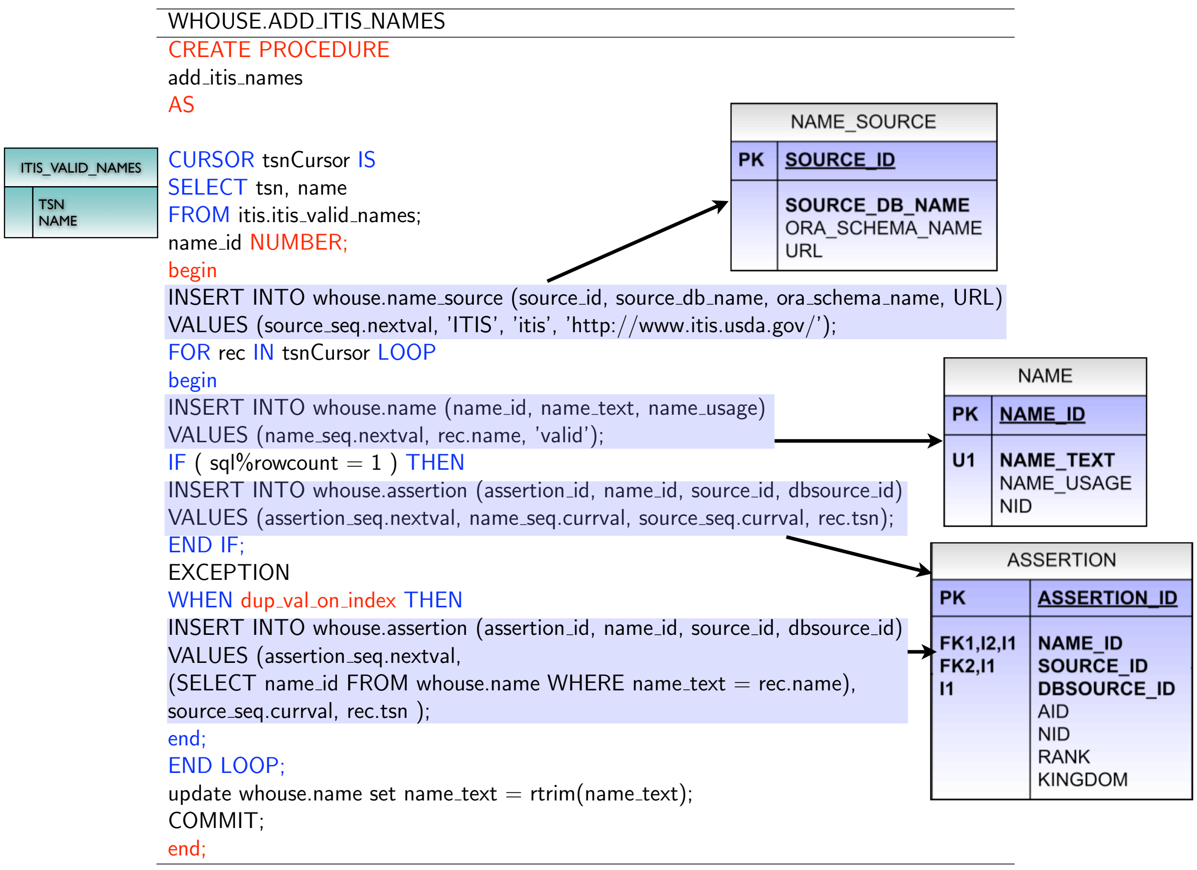
Once ADD_ITIS_NAMES has completed, the second view WHOUSE_ITIS_VALID_MV is built. This view contains all valid name_ids, assertion_ids and the corresponding dbsource_ids that are required in the procedure ADD_ITIS_NODES (Figure 4.4). This procedure loads the precomputed ITIS classification data from the table ITIS_TREE into the table NODE. ITIS_TREE, is populated through the process outlined in Figure 4.5.

This process starts with a Perl script that takes the TSN and Parent_TSN values taken from the TAXONOMIC_UNITS table. The Perl script produces a GML (Graph Markup Language) file, which is used as input into the C++ program GML2NESTEDSQL. A snippet of the GML file is shown below.

```
graph [
comment "This is the ITIS graph"
directed 1
node [id 999999 label "999999" ]
node [id 202423 label "202423"]
node [id 46861 label "46861"]
node [id 46862 label "46862"]
...
...
```

The text file produced from this program is then loaded into the table using SQL*Loader.

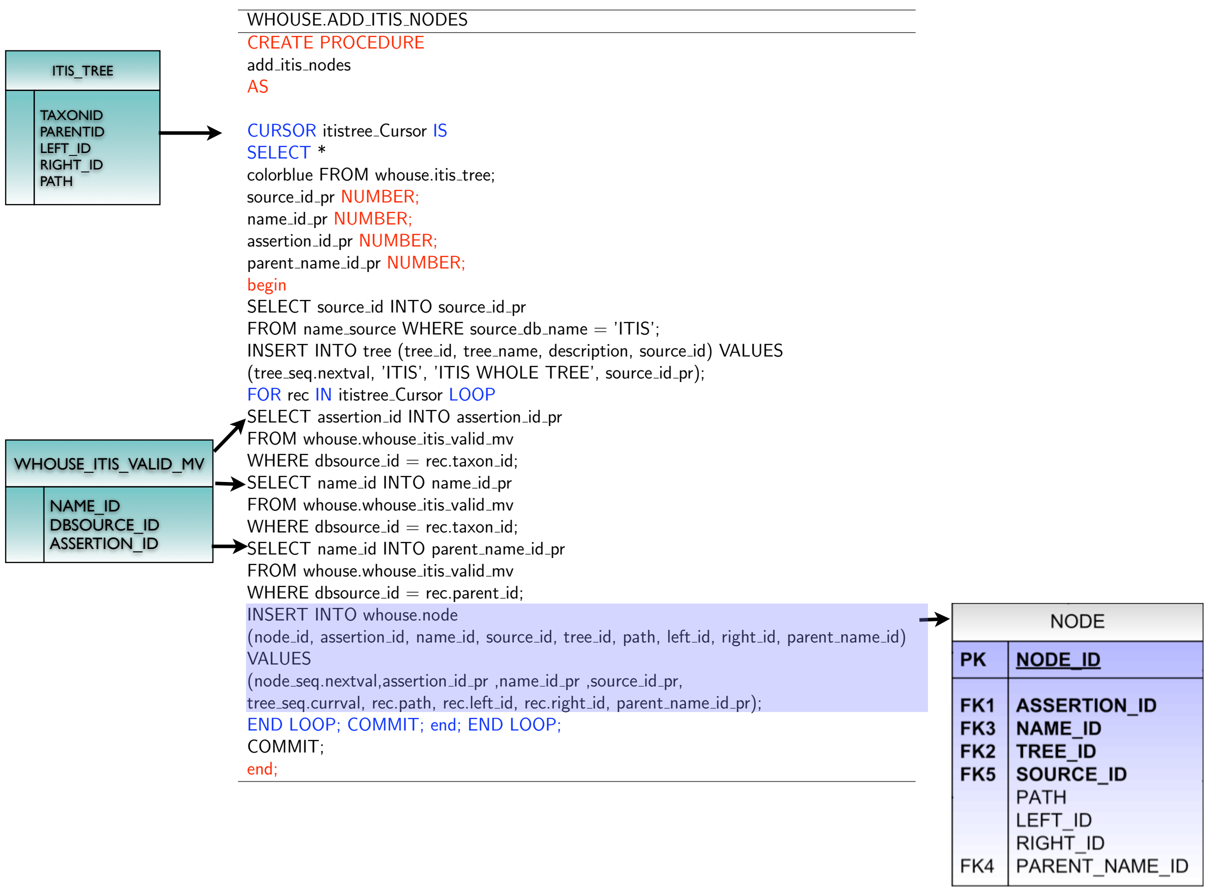
Synonyms and vernaculars are loaded into the global schema using the procedures ADD_ITIS_SYNONYMS and ADD_ITIS_VERNACULARS. The procedure ADD_ITIS_VERNACULARS (Figure 4.6) takes data from the VERNACULARS table, using the TSN and Vernacular_name attributes. In this table the TSN is the TSN of the associated valid name (primary key used in TAXONOMIC UNITS), the vernacular name does not have a TSN in the ITIS tables. In TCl-Db every names source id is stored in the ASSERTION table. For ITIS vernaculars it is the TSN of the valid names that is stored. Synonyms within ITIS are stored in the SYNONYM_LINKS table, and the TAXONOMIC_UNITS table. Synonym names are loaded with



```
WHOUSE.ADD_ITIS_NAMES
CREATE PROCEDURE
add_itis_names
AS

CURSOR tsnCursor IS
SELECT tsn, name
FROM itis.itis_valid_names;
name_id NUMBER;
begin
INSERT INTO whouse.name_source (source_id, source_db_name, ora_schema_name, URL)
VALUES (source_seq.nextval, 'ITIS', 'itis', 'http://www.itis.usda.gov/');
FOR rec IN tsnCursor LOOP
begin
INSERT INTO whouse.name (name_id, name_text, name_usage)
VALUES (name_seq.nextval, rec.name, 'valid');
IF ( sql%rowcount = 1 ) THEN
INSERT INTO whouse.assertion (assertion_id, name_id, source_id, dbsource_id)
VALUES (assertion_seq.nextval, name_seq.currval, source_seq.currval, rec.tsn);
END IF;
EXCEPTION
WHEN dup_val_on_index THEN
INSERT INTO whouse.assertion (assertion_id, name_id, source_id, dbsource_id)
VALUES (assertion_seq.nextval,
(SELECT name_id FROM whouse.name WHERE name_text = rec.name),
source_seq.currval, rec.tsn );
end;
END LOOP;
update whouse.name set name_text = rtrim(name_text);
COMMIT;
end;
```

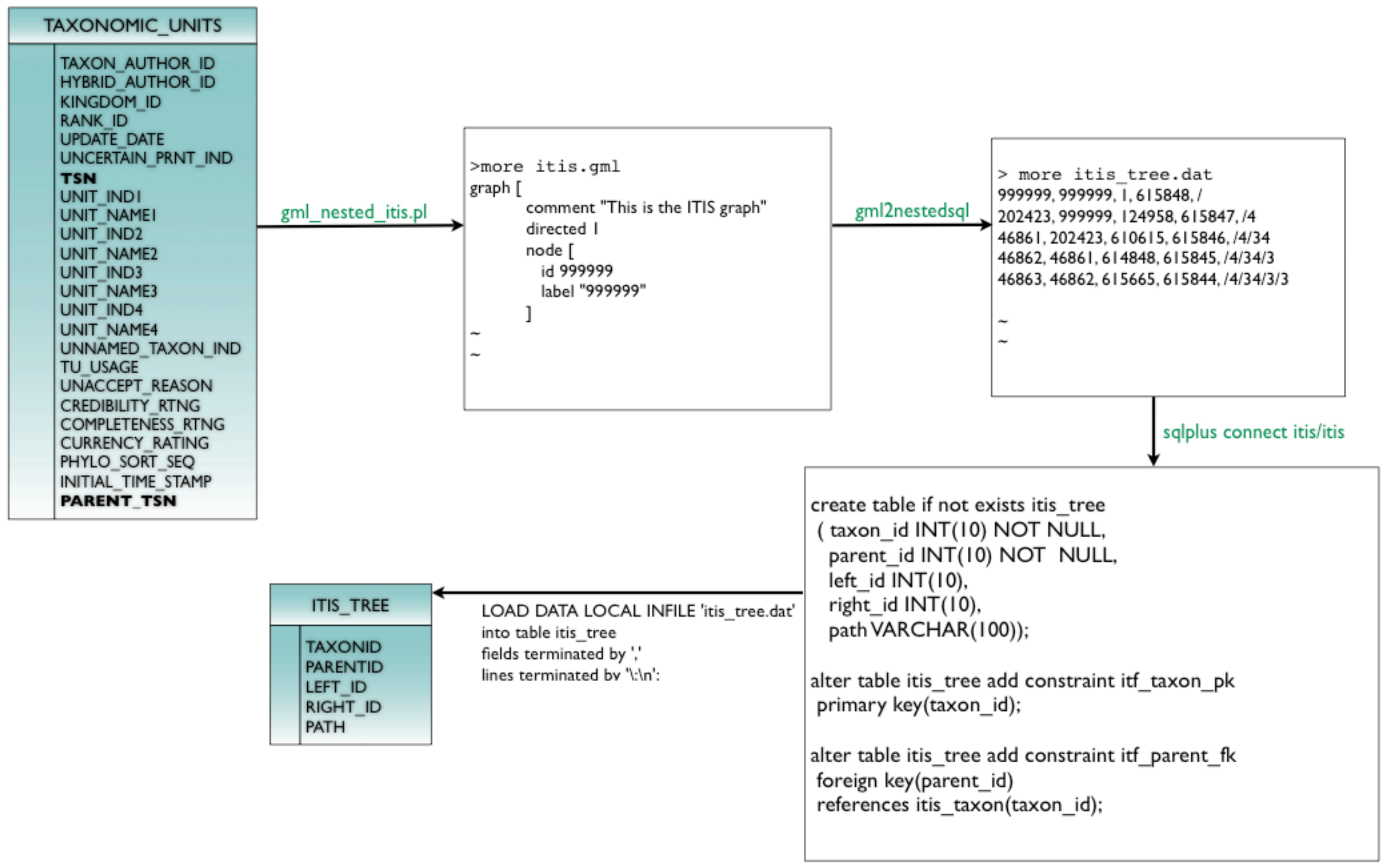
Figure 4.3: The procedure ADD_ITIS_NAMES is run first. This procedure takes data from the view ITIS_VALID_NAMES and fills the tables NAME_SOURCE, NAME and ASSERTION. The procedure is run using the command `execute add_itis_names` at the SQL command prompt.

the procedure ADD_ITIS_SYNONYMS (Figure 4.7). In TAXONOMIC_UNITS synonyms are distinguished from valid names through the tu_usage attribute. Synonyms have the value 'invalid' or 'not accepted'. These names are linked to their valid or accepted name through the value of tsn_accepted.



```
WHOUSE.ADD_ITIS_NODES
CREATE PROCEDURE
add_itis_nodes
AS

CURSOR itistree_Cursor IS
SELECT *
colorblue FROM whouse.itis_tree;
source_id_pr NUMBER;
name_id_pr NUMBER;
assertion_id_pr NUMBER;
parent_name_id_pr NUMBER;
begin
SELECT source_id INTO source_id_pr
FROM name_source WHERE source_db_name = 'ITIS';
INSERT INTO tree (tree_id, tree_name, description, source_id) VALUES
(tree_seq.nextval, 'ITIS', 'ITIS WHOLE TREE', source_id_pr);
FOR rec IN itistree_Cursor LOOP
SELECT assertion_id INTO assertion_id_pr
FROM whouse.whouse_itis_valid_mv
WHERE dbsource_id = rec.taxon_id;
SELECT name_id INTO name_id_pr
FROM whouse.whouse_itis_valid_mv
WHERE dbsource_id = rec.taxon_id;
SELECT name_id INTO parent_name_id_pr
FROM whouse.whouse_itis_valid_mv
WHERE dbsource_id = rec.parent_id;
INSERT INTO whouse.node
(node_id, assertion_id, name_id, source_id, tree_id, path, left_id, right_id, parent_name_id)
VALUES
(node_seq.nextval,assertion_id_pr ,name_id_pr ,source_id_pr,
tree_seq.currval, rec.path, rec.left_id, rec.right_id, parent_name_id_pr);
END LOOP; COMMIT; end; END LOOP;
COMMIT;
end;
```

Figure 4.4: This procedure is run using the command "execute add_itis_nodes" at the SQL command prompt, once the procedure ADD_ITIS_NAMES has completed.



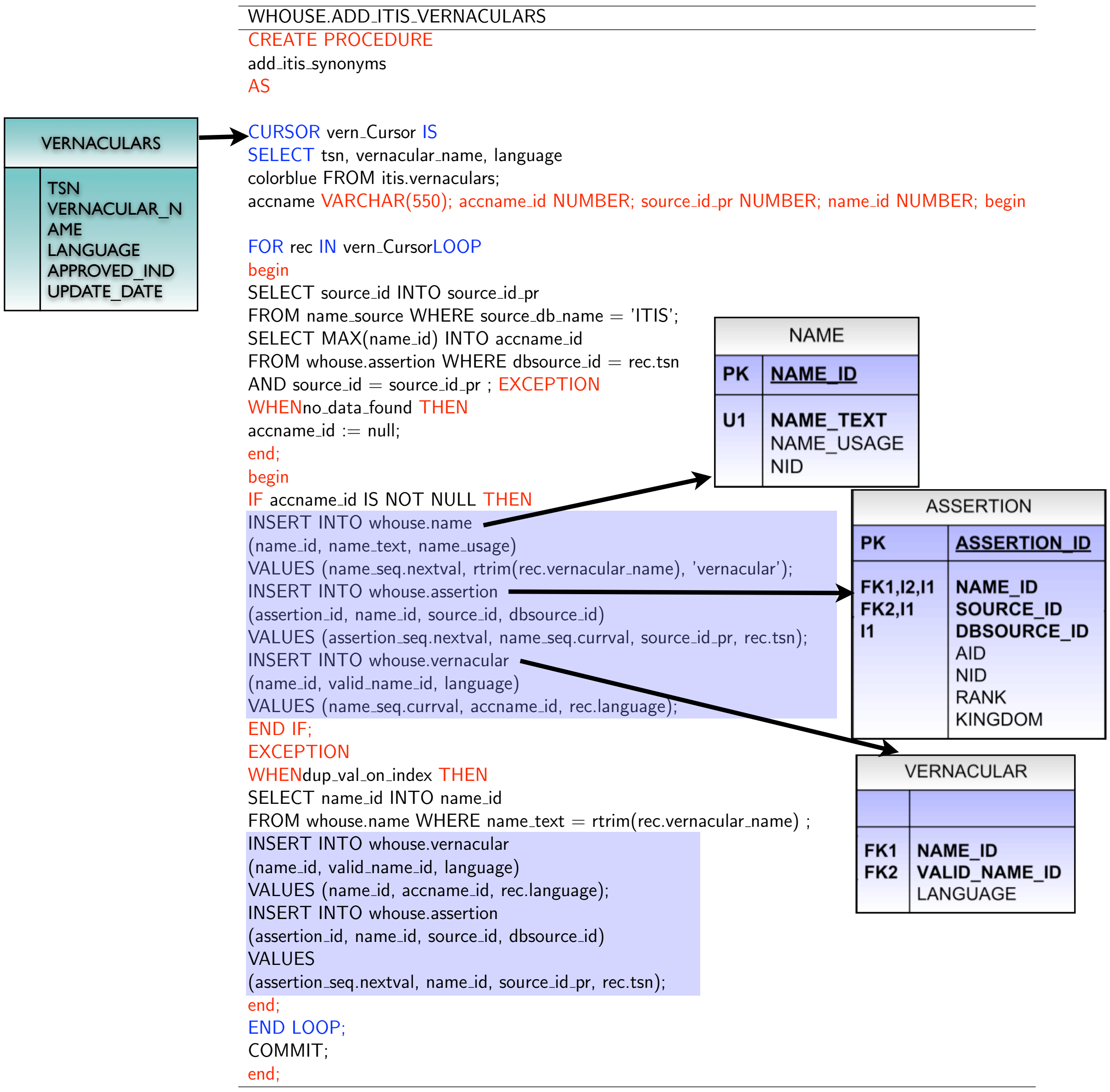
```
>more itis.gml
graph [
        comment "This is the ITIS graph"
        directed 1
        node [
          id 999999
          label "999999"
        ]
~
~
```

```
> more itis_tree.dat
999999, 999999, 1, 615848, /
202423, 999999, 124958, 615847, /4
46861, 202423, 610615, 615846, /4/34
46862, 46861, 614848, 615845, /4/34/3
46863, 46862, 615665, 615844, /4/34/3/3

~
~
```

```
create table if not exists itis_tree
 ( taxon_id INT(10) NOT NULL,
   parent_id INT(10) NOT  NULL,
   left_id INT(10),
   right_id INT(10),
   path VARCHAR(100));

alter table itis_tree add constraint itf_taxon_pk
 primary key(taxon_id);

alter table itis_tree add constraint itf_parent_fk
 foreign key(parent_id)
 references itis_taxon(taxon_id);
```

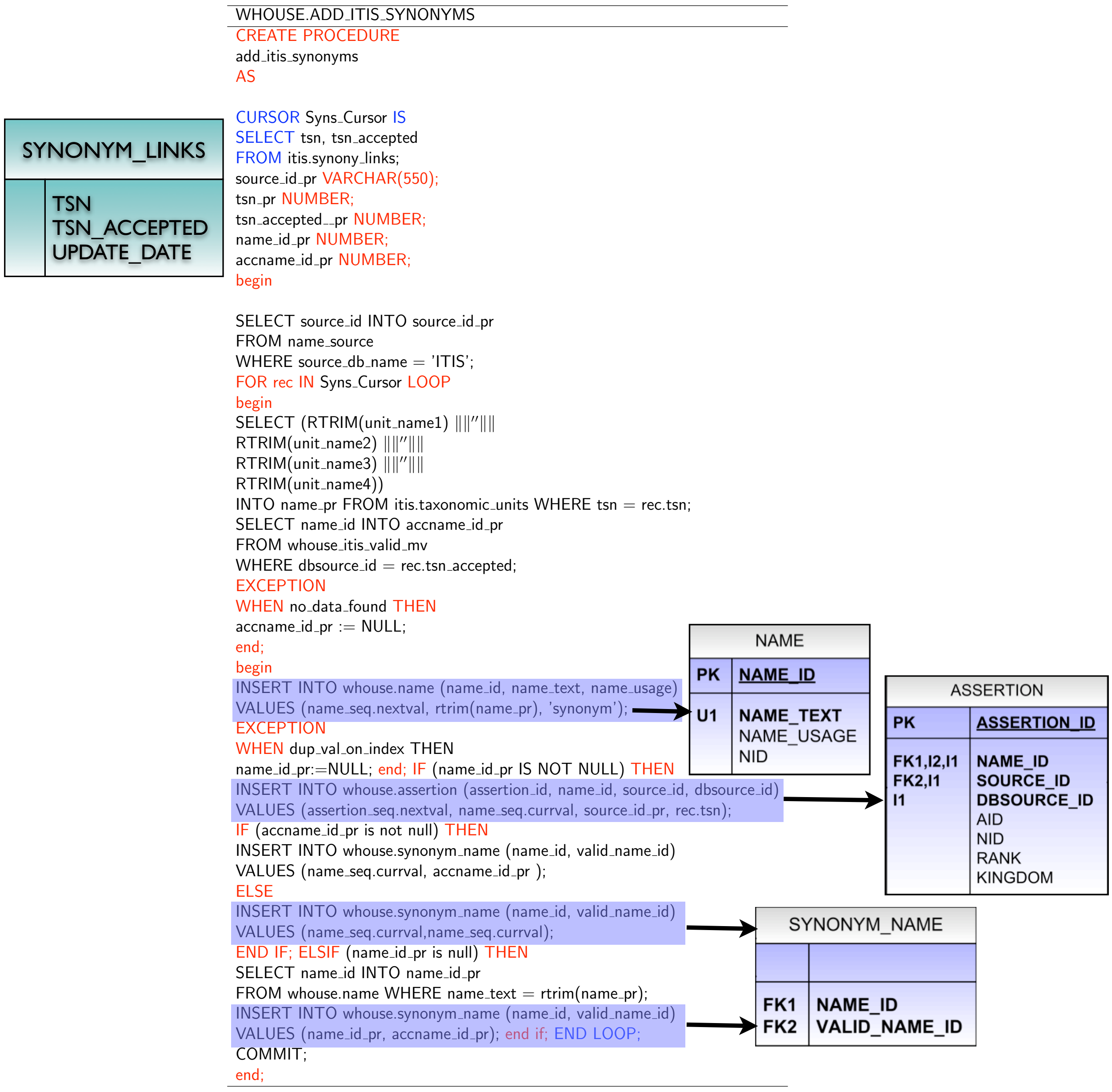
```
LOAD DATA LOCAL INFILE 'itis_tree.dat'
into table itis_tree
fields terminated by ','
lines terminated by '\:\n':
```

Figure 4.5: Algorithm used to build the tree data.



```
WHOUSE.ADD_ITIS_VERNACULARS
CREATE PROCEDURE
add_itis_synonyms
AS

CURSOR vern_Cursor IS
SELECT tsn, vernacular_name, language
colorblue FROM itis.vernaculars;
accname VARCHAR(550); accname_id NUMBER; source_id_pr NUMBER; name_id NUMBER; begin

FOR rec IN vern_CursorLOOP
begin
SELECT source_id INTO source_id_pr
FROM name_source WHERE source_db_name = 'ITIS';
SELECT MAX(name_id) INTO accname_id
FROM whouse.assertion WHERE dbsource_id = rec.tsn
AND source_id = source_id_pr ; EXCEPTION
WHENno_data_found THEN
accname_id := null;
end;
begin
IF accname_id IS NOT NULL THEN
INSERT INTO whouse.name
(name_id, name_text, name_usage)
VALUES (name_seq.nextval, rtrim(rec.vernacular_name), 'vernacular');
INSERT INTO whouse.assertion
(assertion_id, name_id, source_id, dbsource_id)
VALUES (assertion_seq.nextval, name_seq.currval, source_id_pr, rec.tsn);
INSERT INTO whouse.vernacular
(name_id, valid_name_id, language)
VALUES (name_seq.currval, accname_id, rec.language);
END IF;
EXCEPTION
WHENdup_val_on_index THEN
SELECT name_id INTO name_id
FROM whouse.name WHERE name_text = rtrim(rec.vernacular_name) ;
INSERT INTO whouse.vernacular
(name_id, valid_name_id, language)
VALUES (name_id, accname_id, rec.language);
INSERT INTO whouse.assertion
(assertion_id, name_id, source_id, dbsource_id)
VALUES
(assertion_seq.nextval, name_id, source_id_pr, rec.tsn);
end;
END LOOP;
COMMIT;
end;
```

Figure 4.6: Procedure ADD_ITIS_VERNACULARS. This procedure should be run after all valid names have been loaded using the ADD_ITIS_NAMES procedure.



```
WHOUSE.ADD_ITIS_SYNONYMS
CREATE PROCEDURE
add_itis_synonyms
AS

CURSOR Syns_Cursor IS
SELECT tsn, tsn_accepted
FROM itis.synony_links;
source_id_pr VARCHAR(550);
tsn_pr NUMBER;
tsn_accepted__pr NUMBER;
name_id_pr NUMBER;
accname_id_pr NUMBER;
begin

SELECT source_id INTO source_id_pr
FROM name_source
WHERE source_db_name = 'ITIS';
FOR rec IN Syns_Cursor LOOP
begin
SELECT (RTRIM(unit_name1) ||||''||||
RTRIM(unit_name2) ||||''||||
RTRIM(unit_name3) ||||''||||
RTRIM(unit_name4))
INTO name_pr FROM itis.taxonomic_units WHERE tsn = rec.tsn;
SELECT name_id INTO accname_id_pr
FROM whouse_itis_valid_mv
WHERE dbsource_id = rec.tsn_accepted;
EXCEPTION
WHEN no_data_found THEN
accname_id_pr := NULL;
end;
begin
INSERT INTO whouse.name (name_id, name_text, name_usage)
VALUES (name_seq.nextval, rtrim(name_pr), 'synonym');
EXCEPTION
WHEN dup_val_on_index THEN
name_id_pr:=NULL; end; IF (name_id_pr IS NOT NULL) THEN
INSERT INTO whouse.assertion (assertion_id, name_id, source_id, dbsource_id)
VALUES (assertion_seq.nextval, name_seq.currval, source_id_pr, rec.tsn);
IF (accname_id_pr is not null) THEN
INSERT INTO whouse.synonym_name (name_id, valid_name_id)
VALUES (name_seq.currval, accname_id_pr );
ELSE
INSERT INTO whouse.synonym_name (name_id, valid_name_id)
VALUES (name_seq.currval,name_seq.currval);
END IF; ELSIF (name_id_pr is null) THEN
SELECT name_id INTO name_id_pr
FROM whouse.name WHERE name_text = rtrim(name_pr);
INSERT INTO whouse.synonym_name (name_id, valid_name_id)
VALUES (name_id_pr, accname_id_pr); end if; END LOOP;
COMMIT;
end;
```

Figure 4.7: Procedure ADD_ITIS_SYNONYMS. This procedure should be run after all valid names have been loaded using the ADD_ITIS_NAMES procedure.

4.3 NCBI

The National Center for Biotechnology Information (NCBI) (Federhen et.al, 2005) taxonomy was originally built to enable taxonomic indexing in their Entrez system and the Genbank sequence database. The NCBI taxonomy can now be downloaded as a separate database and has been adopted by most other sequence databases. The data are provided as flat file downloads. The download includes 7 tab delimited text files. In this work a schema was created for the NCBI data in which the file structures were replicated into tables and the data were loaded using SQLLDR.

4.3.1 Schema mapping and Integration

The architecture of the NCBI mapping and integration is summarised in Figure 4.8.

The first step in migration identifies scientific names in the NCBI tables, from which the NCBI classification tree data are collected. A perl script uses the table NCBI_NODES (see Figure 4.9) from which the TAX_ID and PARENT_TAX_ID are used to build the nested set and path data. These data are transformed, using the same scripts as ITIS above and loaded into into the table NCBI_TREE. The table NCBI_NAMES holds taxon names within NAME_TEXT attribute. Scientific names were distinguished from synonyms and vernaculars using the NAME_CLASS attribute in the same table. These data were extracted and initially transformed into three materialized views shown in Figure 4.9.

The first view built is NCBI_SCI_NAMES_MV, using the source tables NCBI_NAME and NCBI_NODES. This view is then used to build NCBI_ONLY_NAMES_MV by comparing the NCBI names to all names that are already loaded in the warehouse. Since the ITIS database was loaded first, the view NCBI_ITIS_NAMES_MV stores the names common to both ITIS and NCBI that have already been loaded into the schema. Names in this view add NCBI assertions for names that already exist in TCl-Db..

The first procedure run is ADD_NCBI_NAMES (see Figure 4.10). This loads the tables NAME_SOURCE, NAME and ASSERTION. Once this procedure is finished, the names that have just been loaded now have TCl-Db attributes NAME_ID, ASSERTION_ID and the DBSOURCE_ID. These are identified and stored in another materialized view, WHOUSE_NCBI_VALID_MV. This view is used to speed up the next data load, ADD_NCBI_NODES (see Figure 4.11). Synonyms and vernaculars are added using the procedures ADD_NCBI_SYNONYMS(see Figure 4.12) and ADD_NCBI_VERNACULARS, following a similar process as the ITIS load.

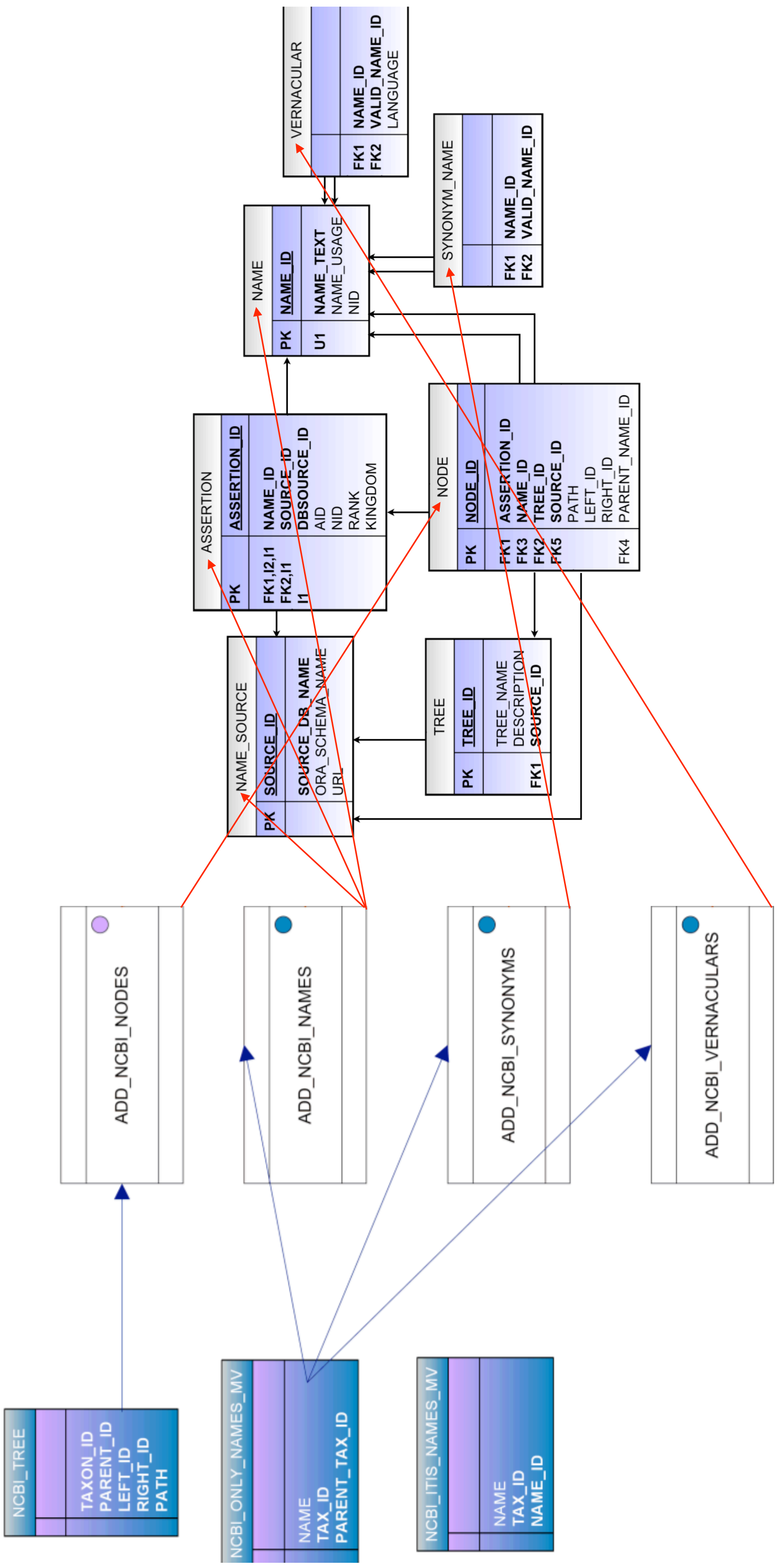
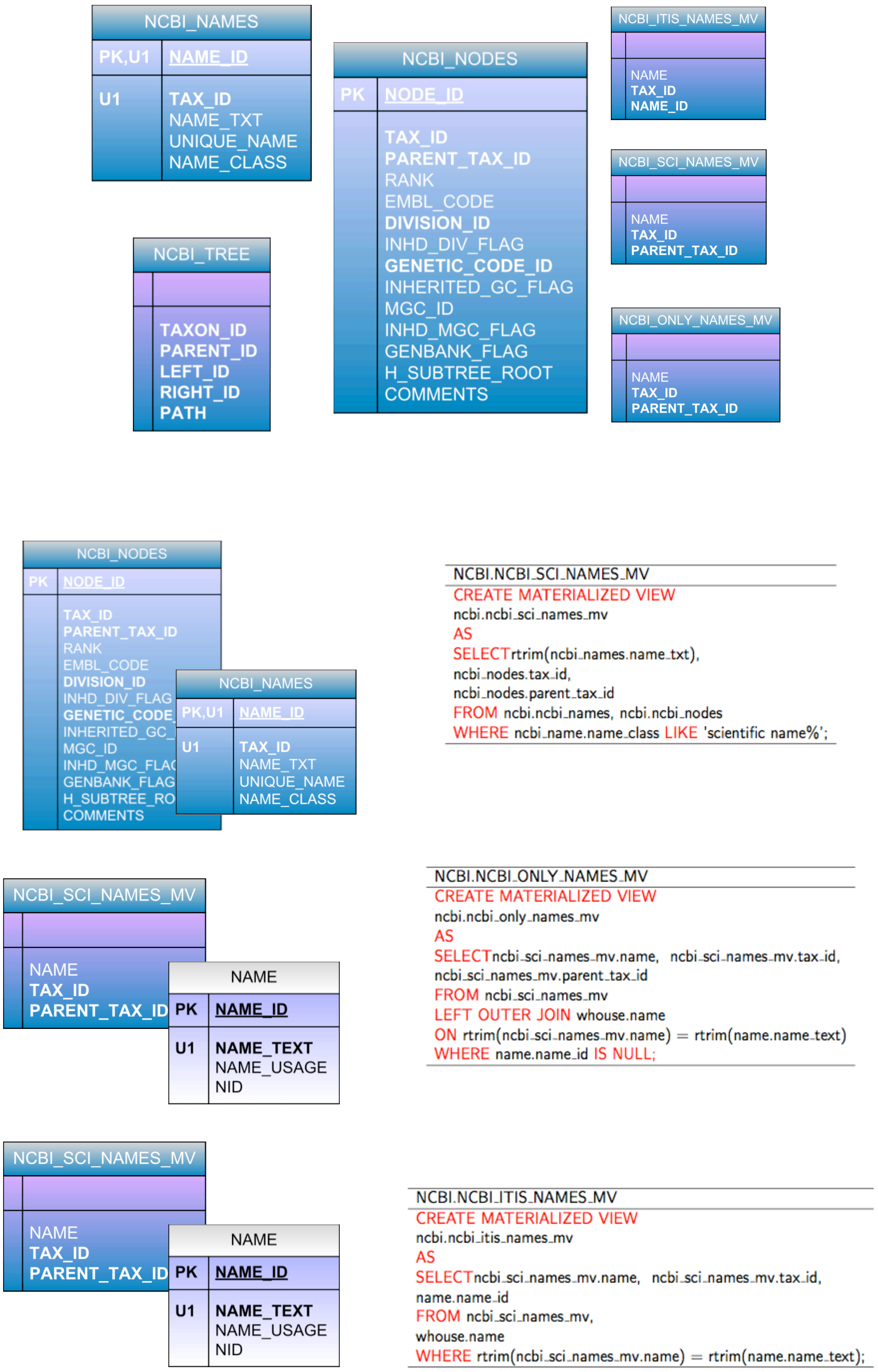


Figure 4.8: Schema mapping NCBI to TCl-Db.

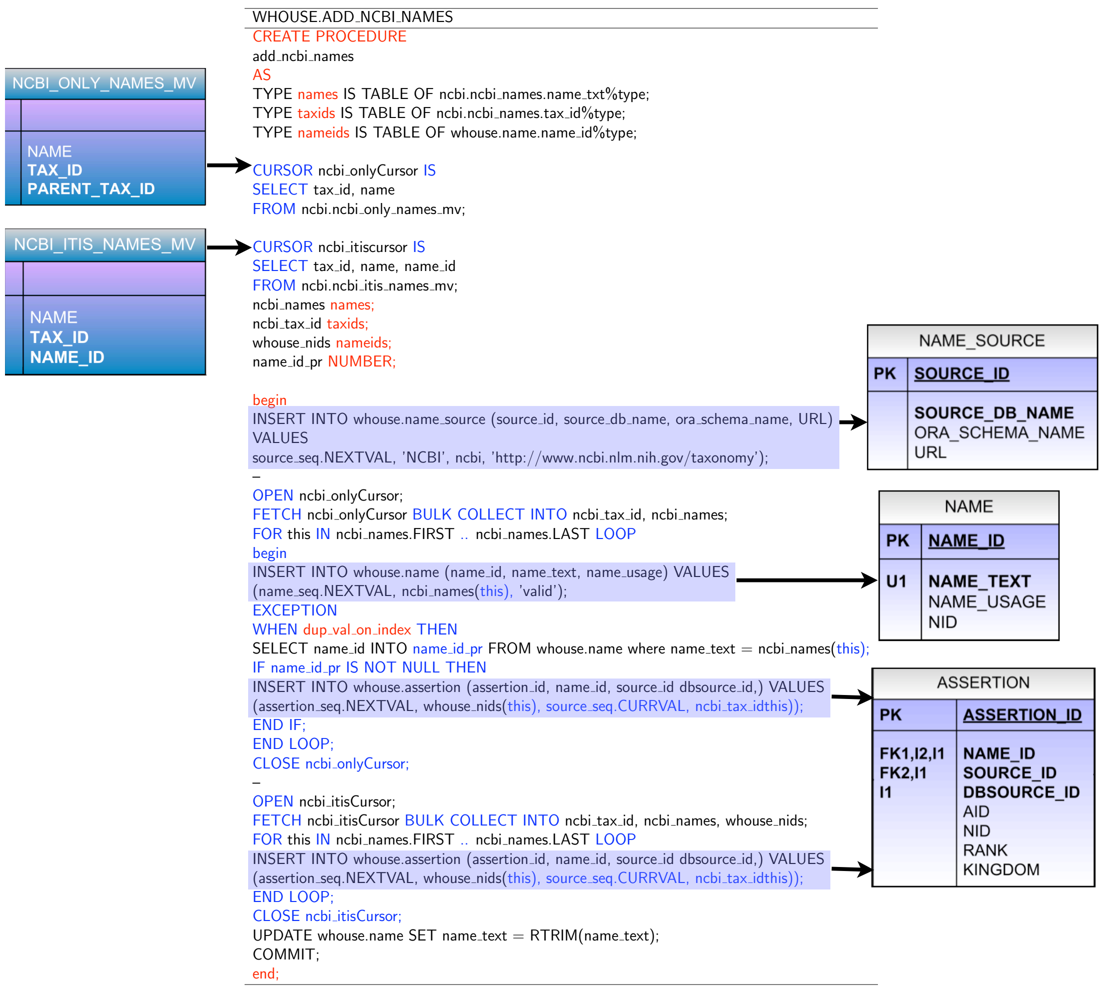


```
NCBI.NCBI_SCI_NAMES_MV
CREATE MATERIALIZED VIEW
ncbi.ncbi_sci_names_mv
AS
SELECTrtrim(ncbi_names.name_txt),
ncbi_nodes.tax_id,
ncbi_nodes.parent_tax_id
FROM ncbi.ncbi_names, ncbi.ncbi_nodes
WHERE ncbi_name.name_class LIKE 'scientific name%';
```

```
NCBI.NCBI_ONLY_NAMES_MV
CREATE MATERIALIZED VIEW
ncbi.ncbi_only_names_mv
AS
SELECTncbi_sci_names_mv.name,  ncbi_sci_names_mv.tax_id,
ncbi_sci_names_mv.parent_tax_id
FROM ncbi_sci_names_mv
LEFT OUTER JOIN whouse.name
ON rtrim(ncbi_sci_names_mv.name) = rtrim(name.name_text)
WHERE name.name_id IS NULL;
```

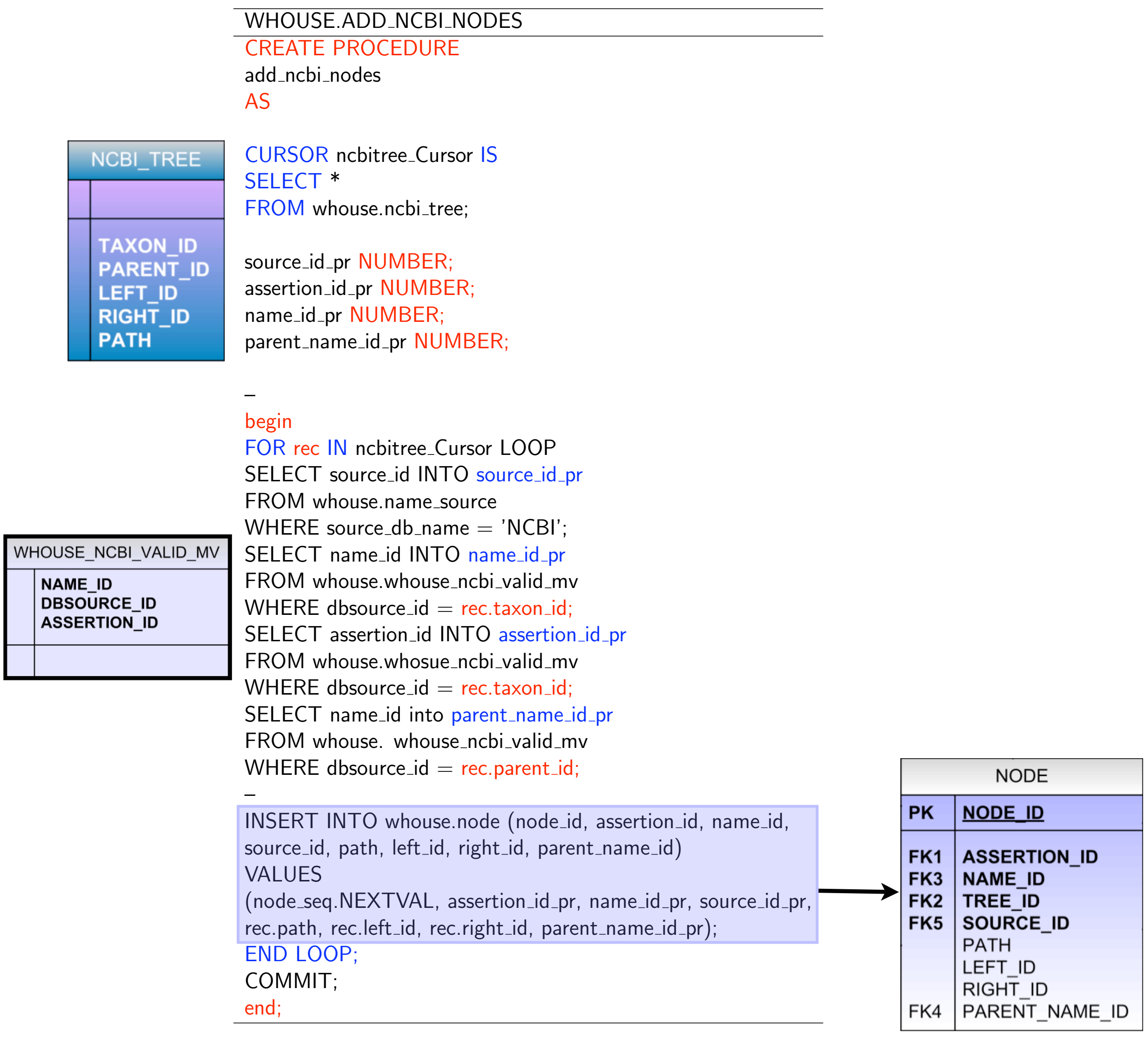
```
NCBI.NCBI_ITIS_NAMES_MV
CREATE MATERIALIZED VIEW
ncbi.ncbi_itis_names_mv
AS
SELECTncbi_sci_names_mv.name,  ncbi_sci_names_mv.tax_id,
name.name_id
FROM ncbi_sci_names_mv,
whouse.name
WHERE rtrim(ncbi_sci_names_mv.name) = rtrim(name.name_text);
```

Figure 4.9: The NCBI tables and views that were built during schema mapping.



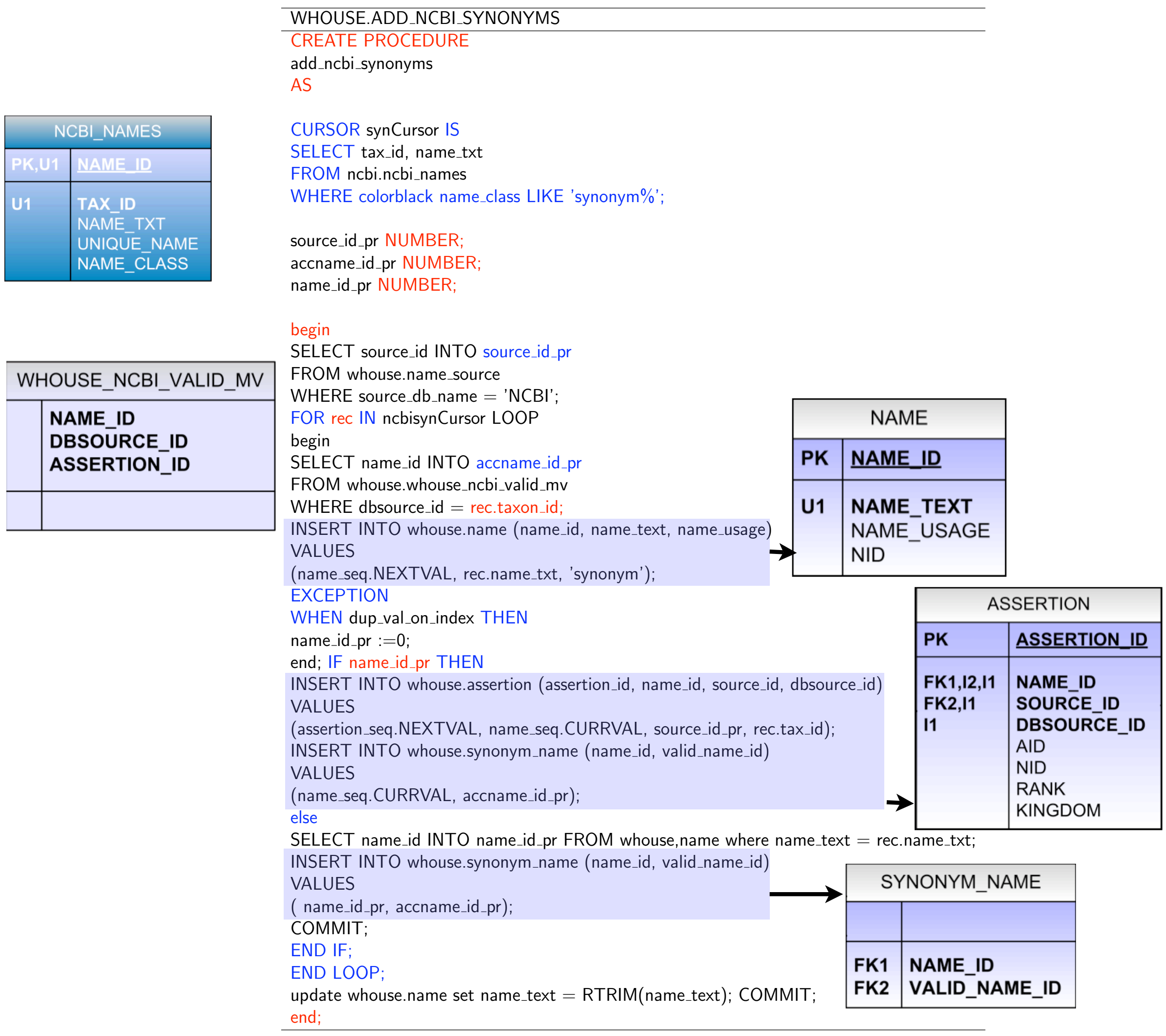
```
WHOUSE.ADD_NCBI_NAMES
CREATE PROCEDURE
add_ncbi_names
AS
TYPE names IS TABLE OF ncbi.ncbi_names.name_txt%type;
TYPE taxids IS TABLE OF ncbi.ncbi_names.tax_id%type;
TYPE nameids IS TABLE OF whouse.name.name_id%type;

CURSOR ncbi_onlyCursor IS
SELECT tax_id, name
FROM ncbi.ncbi_only_names_mv;

CURSOR ncbi_itiscursor IS
SELECT tax_id, name, name_id
FROM ncbi.ncbi_itis_names_mv;
ncbi_names names;
ncbi_tax_id taxids;
whouse_nids nameids;
name_id_pr NUMBER;

begin
INSERT INTO whouse.name_source (source_id, source_db_name, ora_schema_name, URL)
VALUES
source_seq.NEXTVAL, 'NCBI', ncbi, 'http://www.ncbi.nlm.nih.gov/taxonomy');
–
OPEN ncbi_onlyCursor;
FETCH ncbi_onlyCursor BULK COLLECT INTO ncbi_tax_id, ncbi_names;
FOR this IN ncbi_names.FIRST .. ncbi_names.LAST LOOP
begin
INSERT INTO whouse.name (name_id, name_text, name_usage) VALUES
(name_seq.NEXTVAL, ncbi_names(this), 'valid');
EXCEPTION
WHEN dup_val_on_index THEN
SELECT name_id INTO name_id_pr FROM whouse.name where name_text = ncbi_names(this);
IF name_id_pr IS NOT NULL THEN
INSERT INTO whouse.assertion (assertion_id, name_id, source_id dbsource_id,) VALUES
(assertion_seq.NEXTVAL, whouse_nids(this), source_seq.CURRVAL, ncbi_tax_idthis));
END IF;
END LOOP;
CLOSE ncbi_onlyCursor;
–
OPEN ncbi_itisCursor;
FETCH ncbi_itisCursor BULK COLLECT INTO ncbi_tax_id, ncbi_names, whouse_nids;
FOR this IN ncbi_names.FIRST .. ncbi_names.LAST LOOP
INSERT INTO whouse.assertion (assertion_id, name_id, source_id dbsource_id,) VALUES
(assertion_seq.NEXTVAL, whouse_nids(this), source_seq.CURRVAL, ncbi_tax_idthis));
END LOOP;
CLOSE ncbi_itisCursor;
UPDATE whouse.name SET name_text = RTRIM(name_text);
COMMIT;
end;
```

Figure 4.10: The procedure ADD_NCBI_NAMES is run first. This procedure takes data from the views shown in Figure 4.9 and fills the tables NAME and ASSERTION. The procedure is run using the command "execute add_ncbi_names" at the SQL command prompt.



```
WHOUSE.ADD_NCBI_NODES
CREATE PROCEDURE
add_ncbi_nodes
AS

CURSOR ncbitree_Cursor IS
SELECT *
FROM whouse.ncbi_tree;

source_id_pr NUMBER;
assertion_id_pr NUMBER;
name_id_pr NUMBER;
parent_name_id_pr NUMBER;

–
begin
FOR rec IN ncbitree_Cursor LOOP
SELECT source_id INTO source_id_pr
FROM whouse.name_source
WHERE source_db_name = 'NCBI';
SELECT name_id INTO name_id_pr
FROM whouse.whouse_ncbi_valid_mv
WHERE dbsource_id = rec.taxon_id;
SELECT assertion_id INTO assertion_id_pr
FROM whouse.whosue_ncbi_valid_mv
WHERE dbsource_id = rec.taxon_id;
SELECT name_id into parent_name_id_pr
FROM whouse. whouse_ncbi_valid_mv
WHERE dbsource_id = rec.parent_id;
–
INSERT INTO whouse.node (node_id, assertion_id, name_id,
source_id, path, left_id, right_id, parent_name_id)
VALUES
(node_seq.NEXTVAL, assertion_id_pr, name_id_pr, source_id_pr,
rec.path, rec.left_id, rec.right_id, parent_name_id_pr);
END LOOP;
COMMIT;
end;
```

Figure 4.11: Procedure ADD_NCBI_NODES is run after ADD_NCBI_NAMES.The NAME_IDS and ASSERTION_ID are taken from the view sc whouse_ncbi_valid_mv.



```
WHOUSE.ADD_NCBI_SYNONYMS
CREATE PROCEDURE
add_ncbi_synonyms
AS

CURSOR synCursor IS
SELECT tax_id, name_txt
FROM ncbi.ncbi_names
WHERE colorblack name_class LIKE 'synonym%';

source_id_pr NUMBER;
accname_id_pr NUMBER;
name_id_pr NUMBER;

begin
SELECT source_id INTO source_id_pr
FROM whouse.name_source
WHERE source_db_name = 'NCBI';
FOR rec IN ncbisynCursor LOOP
begin
SELECT name_id INTO accname_id_pr
FROM whouse.whouse_ncbi_valid_mv
WHERE dbsource_id = rec.taxon_id;
INSERT INTO whouse.name (name_id, name_text, name_usage)
VALUES
(name_seq.NEXTVAL, rec.name_txt, 'synonym');
EXCEPTION
WHEN dup_val_on_index THEN
name_id_pr :=0;
end; IF name_id_pr THEN
INSERT INTO whouse.assertion (assertion_id, name_id, source_id, dbsource_id)
VALUES
(assertion_seq.NEXTVAL, name_seq.CURRVAL, source_id_pr, rec.tax_id);
INSERT INTO whouse.synonym_name (name_id, valid_name_id)
VALUES
(name_seq.CURRVAL, accname_id_pr);
else
SELECT name_id INTO name_id_pr FROM whouse,name where name_text = rec.name_txt;
INSERT INTO whouse.synonym_name (name_id, valid_name_id)
VALUES
( name_id_pr, accname_id_pr);
COMMIT;
END IF;
END LOOP;
update whouse.name set name_text = RTRIM(name_text); COMMIT;
end;
```

Figure 4.12: ADD_NCBI_SYNONYMS . The procedure ADD_NCBI_VERNACULARS is essentially the same, except that the initial query uses "NAME_CLASS LIKE 'VERNACULAR' ".

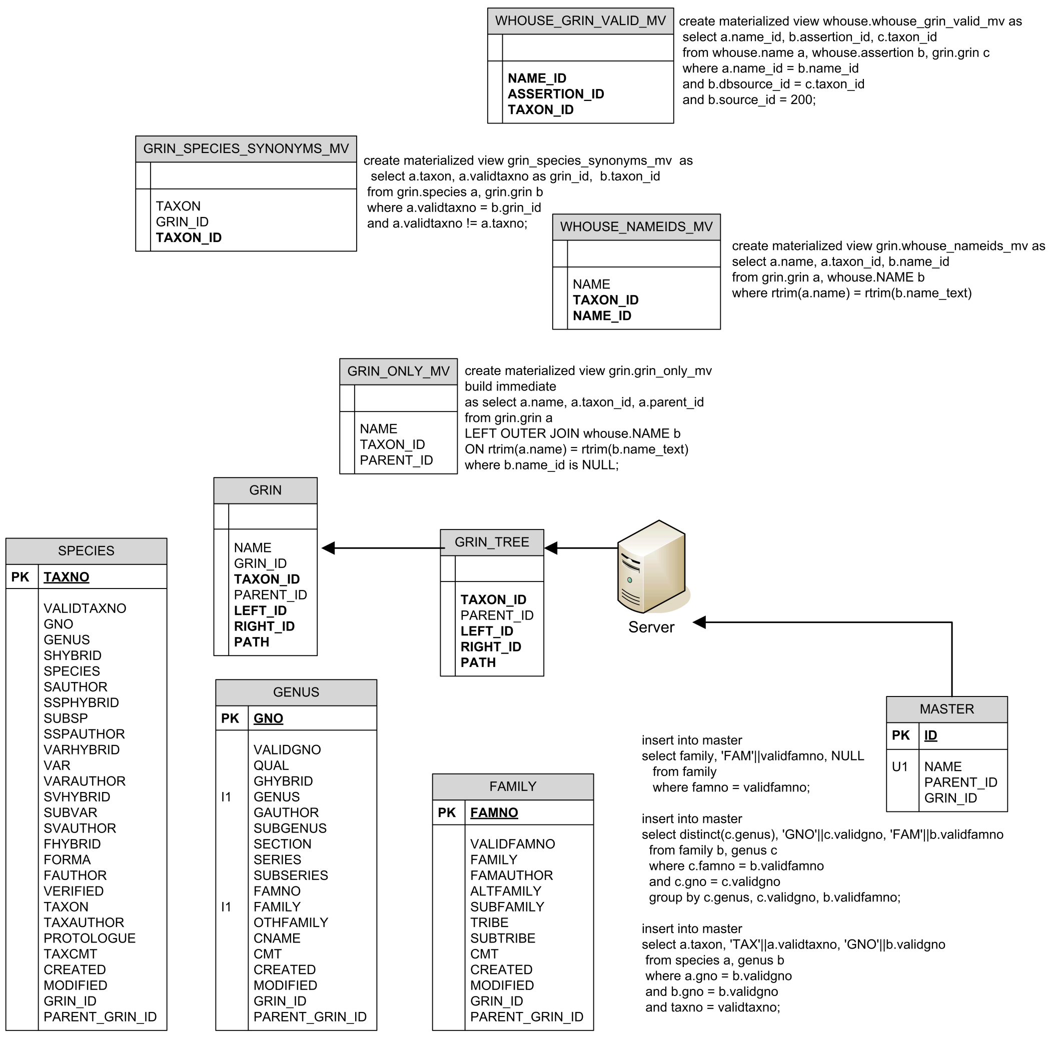
4.4 GRIN

The National Germplasm Information Network (GRIN) (USDA, 2000) contains classification and nomenclature for plant germplasm data held within the (United States) Agricultural Research Service National Plant Germplasm System. The taxonomic data includes scientific names, classification (up to the rank family), synonyms and common names. The taxonomy is curated by experts at the Systematic Botany and Mycology Laboratory in collaboration with world wide experts. Their aim is to reflect the taxonomic opinion of taxonomists from various plant groups and their literature. Data are also taken from floras and checklists. Mostly, the data are guided by expert opinion and, where this is not available, the generally accepted usage. The data downloads are dbf files from Xbase (a desktop database management system like Microsoft Access see *http://xbase.darwinports.com*). The data were extracted from the dbf files and transformed into SQL insert statements. The SQL scripts for each dbf file were loaded into a replicated table structure reflecting the original dbf file.

4.4.1 Schema mapping and Integration

The architecture of the GRIN data integration is summarised in Figure 4.13. The GRIN schema did not conform to standard normalisation or relational rules and the data load was complicated since data items were stored in multiple places and there were several integrity issues that needed to be resolved. These problems were resolved into a master table, with the key data items necessary for TCl-Db. The SPECIES, GENUS and FAMILY table were used to extract hierarchy up to family. The master table was then checked for integrity, one query found thirty-nine species names whose parent name identifiers were missing. Unfortunately the identifiers; SPECIES (TAXNO), GENUS (GNO) and FAMILY (FAMNO) were not unique across the three tables and could not be used. To remedy this, a unique identifier was given to each name as it entered the master table, these were used for the parent child relationships (instead of the identifiers given by GRIN) for the GRIN_TREE table. There were also some data cleaning necessary on the master table to remove disconnected nodes from the tree, these were mostly names that had no parent names i.e. they were assigned as valid names in the tables but the parent names were not valid. In all cases these were leaf nodes in the tree, sub-species names considered valid but the species were invalid.

Once the GRIN table was created, the data were initially transformed into materialized views which were used for the transformation into the TCl-Db schema (see Figures 4.14 and 4.15).



```
create materialized view whouse.whouse_grin_valid_mv as
 select a.name_id, b.assertion_id, c.taxon_id
 from whouse.name a, whouse.assertion b, grin.grin c
 where a.name_id = b.name_id
 and b.dbsource_id = c.taxon_id
 and b.source_id = 200;
```

```
create materialized view grin_species_synonyms_mv  as
  select a.taxon, a.validtaxno as grin_id,  b.taxon_id
 from grin.species a, grin.grin b
 where a.validtaxno = b.grin_id
 and a.validtaxno != a.taxno;
```

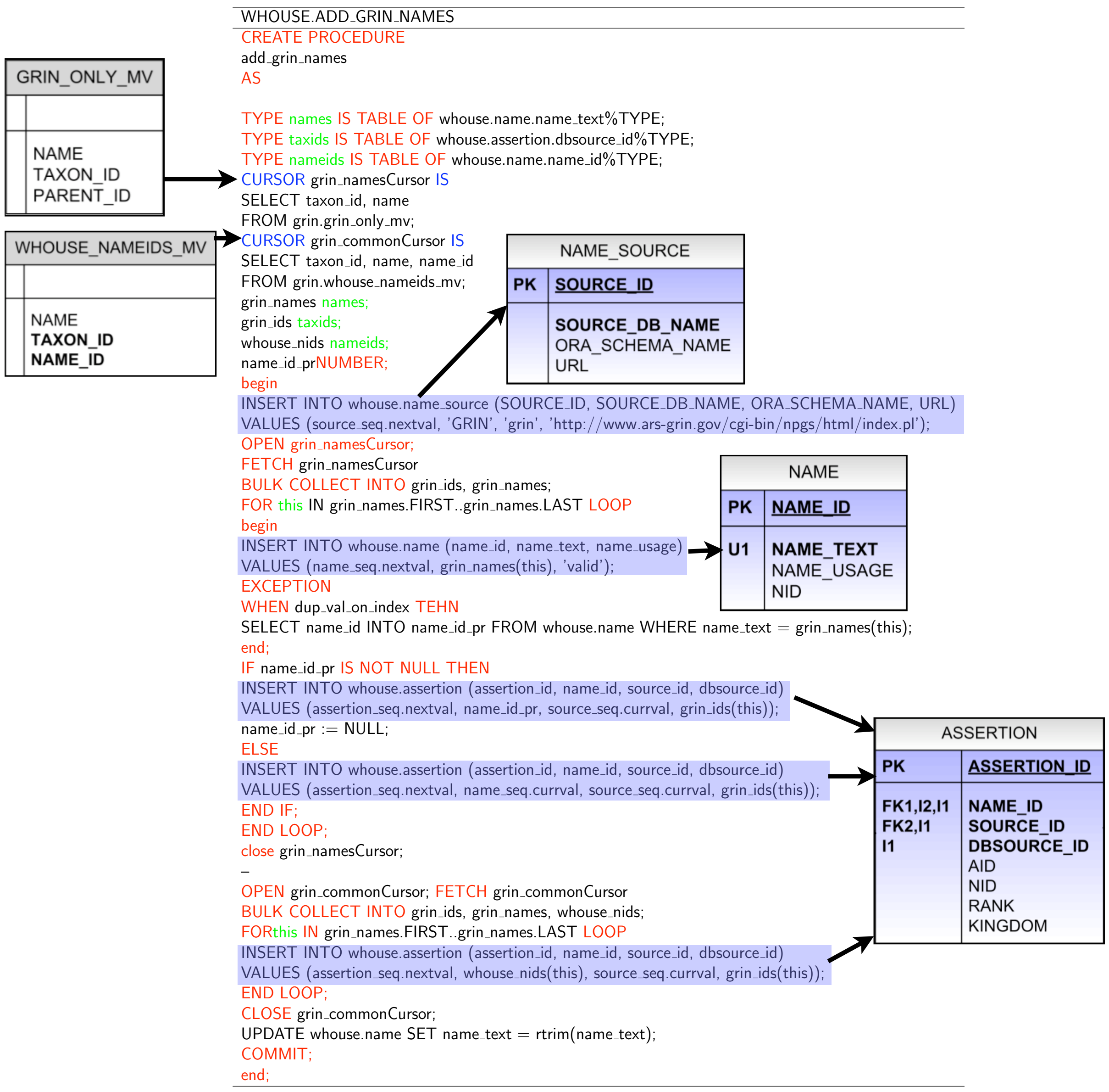
```
create materialized view grin.whouse_nameids_mv as
select a.name, a.taxon_id, b.name_id
from grin.grin a, whouse.NAME b
where rtrim(a.name) = rtrim(b.name_text)
```

```
create materialized view grin.grin_only_mv
build immediate
as select a.name, a.taxon_id, a.parent_id
from grin.grin a
LEFT OUTER JOIN whouse.NAME b
ON rtrim(a.name) = rtrim(b.name_text)
where b.name_id is NULL;
```

```
insert into master
select family, 'FAM'||validfamno, NULL
   from family
   where famno = validfamno;

insert into master
select distinct(c.genus), 'GNO'||c.validgno, 'FAM'||b.validfamno
  from family b, genus c
  where c.famno = b.validfamno
  and c.gno = c.validgno
  group by c.genus, c.validgno, b.validfamno;

insert into master
select a.taxon, 'TAX'||a.validtaxno, 'GNO'||b.validgno
 from species a, genus b
 where a.gno = b.validgno
 and b.gno = b.validgno
 and taxno = validtaxno;
```

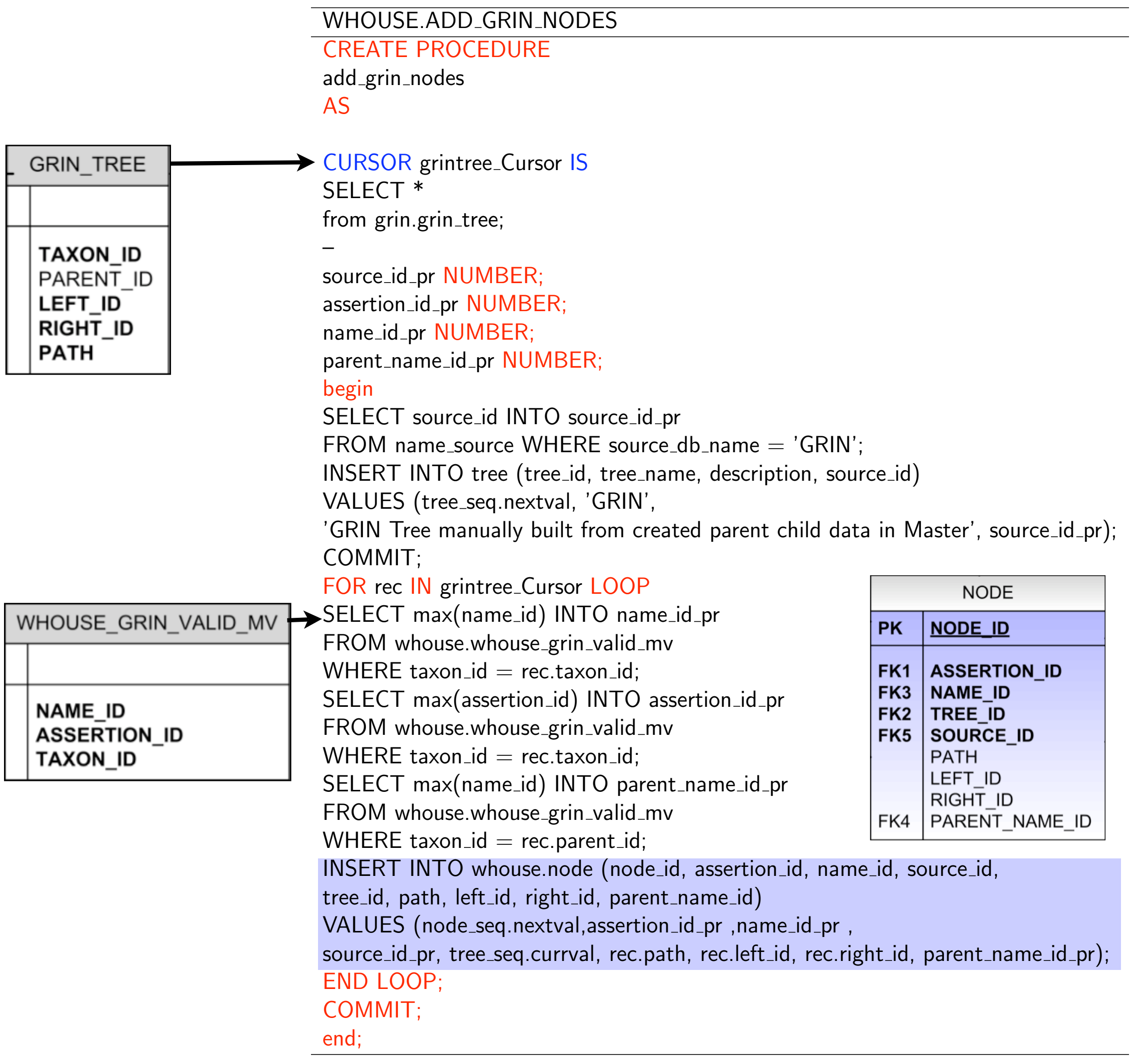
Figure 4.13: Overview of the GRIN data migration.

Synonyms were extracted for species data using the GRIN table and the original GRIN SPECIES table. Synonyms were stored in the schema through the primary key TAXNO and candidate key VALIDTAXNO. A valid name would have TAXNO equal to VALIDTAXNO while synonym had a VALIDTAXNO, that did not equate to its own TAXNO. Using the unique identifiers created for the GRIN table, the species synonyms where collected into the materialized view GRIN_SPECIES_SYNONYMS_MV. There were no vernaculars in the GRIN data.



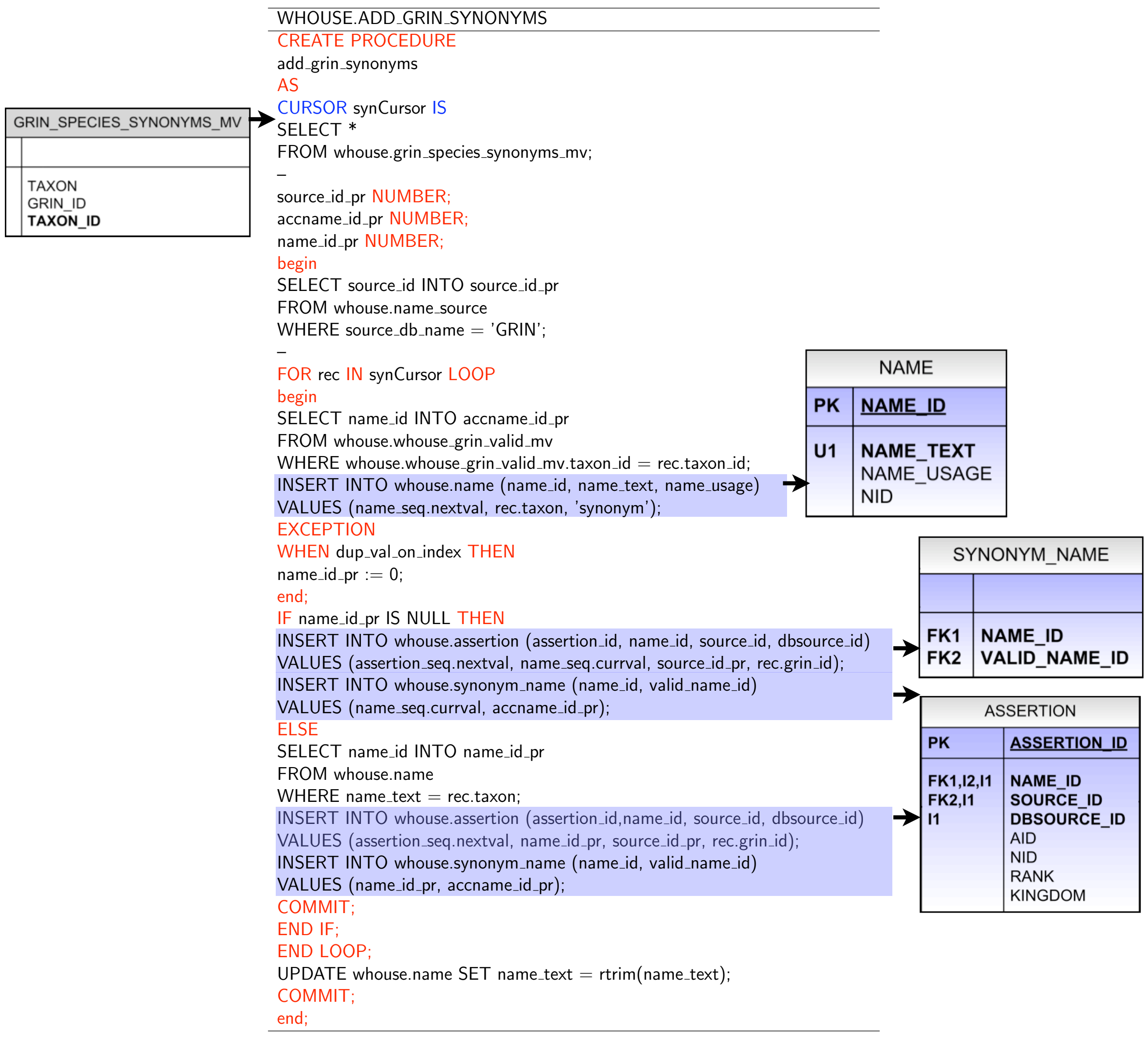
```
WHOUSE.ADD_GRIN_NAMES
CREATE PROCEDURE
add_grin_names
AS

TYPE names IS TABLE OF whouse.name.name_text%TYPE;
TYPE taxids IS TABLE OF whouse.assertion.dbsource_id%TYPE;
TYPE nameids IS TABLE OF whouse.name.name_id%TYPE;
CURSOR grin_namesCursor IS
SELECT taxon_id, name
FROM grin.grin_only_mv;
CURSOR grin_commonCursor IS
SELECT taxon_id, name, name_id
FROM grin.whouse_nameids_mv;
grin_names names;
grin_ids taxids;
whouse_nids nameids;
name_id_prNUMBER;
begin
INSERT INTO whouse.name_source (SOURCE_ID, SOURCE_DB_NAME, ORA_SCHEMA_NAME, URL)
VALUES (source_seq.nextval, 'GRIN', 'grin', 'http://www.ars-grin.gov/cgi-bin/npgs/html/index.pl');
OPEN grin_namesCursor;
FETCH grin_namesCursor
BULK COLLECT INTO grin_ids, grin_names;
FOR this IN grin_names.FIRST..grin_names.LAST LOOP
begin
INSERT INTO whouse.name (name_id, name_text, name_usage)
VALUES (name_seq.nextval, grin_names(this), 'valid');
EXCEPTION
WHEN dup_val_on_index TEHN
SELECT name_id INTO name_id_pr FROM whouse.name WHERE name_text = grin_names(this);
end;
IF name_id_pr IS NOT NULL THEN
INSERT INTO whouse.assertion (assertion_id, name_id, source_id, dbsource_id)
VALUES (assertion_seq.nextval, name_id_pr, source_seq.currval, grin_ids(this));
name_id_pr := NULL;
ELSE
INSERT INTO whouse.assertion (assertion_id, name_id, source_id, dbsource_id)
VALUES (assertion_seq.nextval, name_seq.currval, source_seq.currval, grin_ids(this));
END IF;
END LOOP;
close grin_namesCursor;
–
OPEN grin_commonCursor; FETCH grin_commonCursor
BULK COLLECT INTO grin_ids, grin_names, whouse_nids;
FORthis IN grin_names.FIRST..grin_names.LAST LOOP
INSERT INTO whouse.assertion (assertion_id, name_id, source_id, dbsource_id)
VALUES (assertion_seq.nextval, whouse_nids(this), source_seq.currval, grin_ids(this));
END LOOP;
CLOSE grin_commonCursor;
UPDATE whouse.name SET name_text = rtrim(name_text);
COMMIT;
end;
```

Figure 4.14: Procedure ADD_GRIN_NAMES.



```
WHOUSE.ADD_GRIN_NODES
CREATE PROCEDURE
add_grin_nodes
AS
CURSOR grintree_Cursor IS
SELECT *
from grin.grin_tree;
–
source_id_pr NUMBER;
assertion_id_pr NUMBER;
name_id_pr NUMBER;
parent_name_id_pr NUMBER;
begin
SELECT source_id INTO source_id_pr
FROM name_source WHERE source_db_name = 'GRIN';
INSERT INTO tree (tree_id, tree_name, description, source_id)
VALUES (tree_seq.nextval, 'GRIN',
'GRIN Tree manually built from created parent child data in Master', source_id_pr);
COMMIT;
FOR rec IN grintree_Cursor LOOP
SELECT max(name_id) INTO name_id_pr
FROM whouse.whouse_grin_valid_mv
WHERE taxon_id = rec.taxon_id;
SELECT max(assertion_id) INTO assertion_id_pr
FROM whouse.whouse_grin_valid_mv
WHERE taxon_id = rec.taxon_id;
SELECT max(name_id) INTO parent_name_id_pr
FROM whouse.whouse_grin_valid_mv
WHERE taxon_id = rec.parent_id;
INSERT INTO whouse.node (node_id, assertion_id, name_id, source_id,
tree_id, path, left_id, right_id, parent_name_id)
VALUES (node_seq.nextval,assertion_id_pr ,name_id_pr ,
source_id_pr, tree_seq.currval, rec.path, rec.left_id, rec.right_id, parent_name_id_pr);
END LOOP;
COMMIT;
end;
```

Figure 4.15: Procedure ADD_GRIN_NODES.



```
WHOUSE.ADD_GRIN_SYNONYMS
CREATE PROCEDURE
add_grin_synonyms
AS
CURSOR synCursor IS
SELECT *
FROM whouse.grin_species_synonyms_mv;
–
source_id_pr NUMBER;
accname_id_pr NUMBER;
name_id_pr NUMBER;
begin
SELECT source_id INTO source_id_pr
FROM whouse.name_source
WHERE source_db_name = 'GRIN';
–
FOR rec IN synCursor LOOP
begin
SELECT name_id INTO accname_id_pr
FROM whouse.whouse_grin_valid_mv
WHERE whouse.whouse_grin_valid_mv.taxon_id = rec.taxon_id;
INSERT INTO whouse.name (name_id, name_text, name_usage)
VALUES (name_seq.nextval, rec.taxon, 'synonym');
EXCEPTION
WHEN dup_val_on_index THEN
name_id_pr := 0;
end;
IF name_id_pr IS NULL THEN
INSERT INTO whouse.assertion (assertion_id, name_id, source_id, dbsource_id)
VALUES (assertion_seq.nextval, name_seq.currval, source_id_pr, rec.grin_id);
INSERT INTO whouse.synonym_name (name_id, valid_name_id)
VALUES (name_seq.currval, accname_id_pr);
ELSE
SELECT name_id INTO name_id_pr
FROM whouse.name
WHERE name_text = rec.taxon;
INSERT INTO whouse.assertion (assertion_id,name_id, source_id, dbsource_id)
VALUES (assertion_seq.nextval, name_id_pr, source_id_pr, rec.grin_id);
INSERT INTO whouse.synonym_name (name_id, valid_name_id)
VALUES (name_id_pr, accname_id_pr);
COMMIT;
END IF;
END LOOP;
UPDATE whouse.name SET name_text = rtrim(name_text);
COMMIT;
end;
```

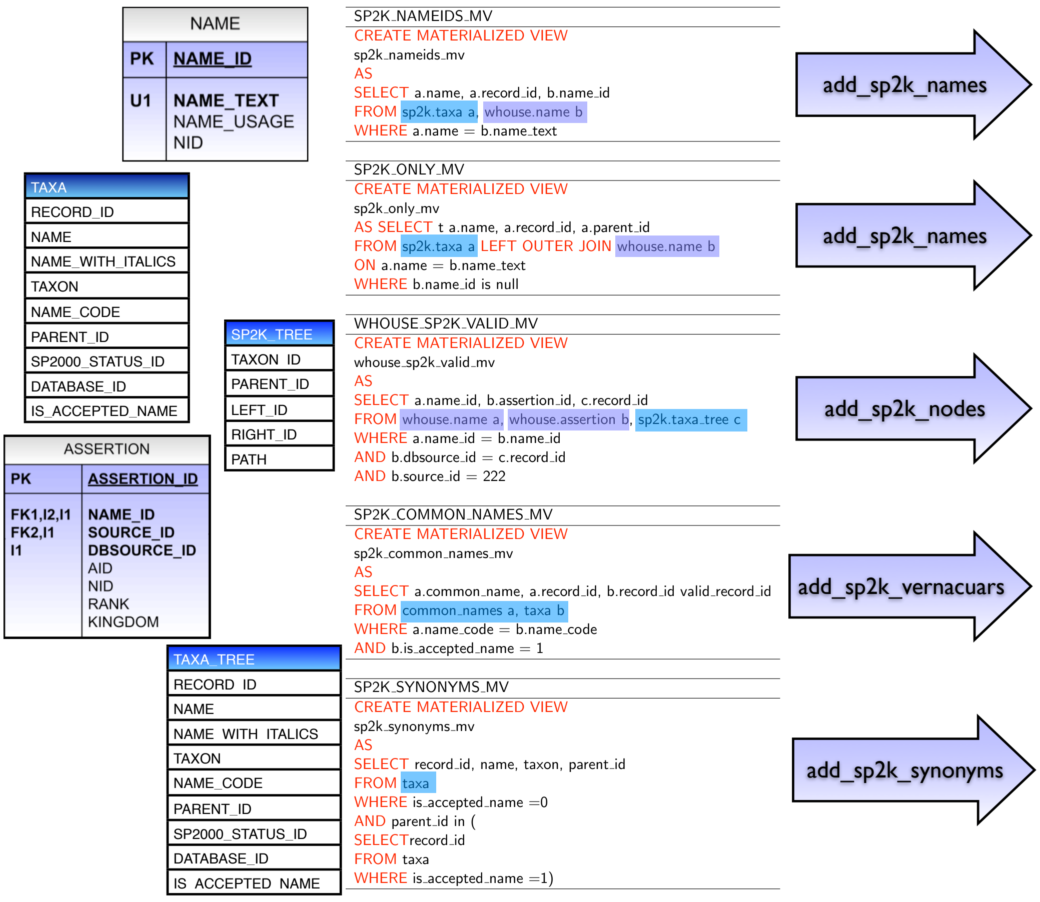
Figure 4.16: Procedure ADD_GRIN_SYNONYMS.

4.5 Sp2000

The Sp2000 system is based on a loosely federated architecture, where the data sources maintain autonomy. Although the architecture of Sp2000 is described as an "autonomous federated system", the system is distributed as a CD so the data are materialised. The annual CD checklist in 2003 was distributed within Microsoft Access. Later versions were moved to MySQL and were much easier to use. The MySQL versions of Sp2000 released in 2005 and 2006 were added to TCl-Db. The MySQL data structure was replicated first into a local installation of MySQL, and the data were then loaded into TCl-Db using SQL dumps.

4.5.1 Schema mapping and Integration

The Sp2000 load uses a layer of materialized views to speed up the data load and also greatly simplify the PL/SQL procedures (Figure 4.17). Names, nodes, synonyms and vernaculars are loaded in much the same way as the other data sources, using specific views. The first view, SP2K_NAMEIDS_MV, gathers the names in Sp2000 that are already in TCl-Db. These data are loaded directly into the ASSERTION table by the ADD_SP2K_NAMES procedure. Names unique to Sp2000 are gathered into the view SP2K_ONLY_MV and are subsequently loaded into the NAME and ASSERTION tables. The table SP2K_TREE is created using a process similar to that outlined in Figure 4.5 for ITIS, using the record_id and parent_id attributes in the TAXA_TREE table. These data are loaded into TCl-Db, using data gathered into the materialized view, sp2k_valid_mv which is built once the add_sp2k_names procedure has completed. In Sp2000 synonyms are stored in the TAXA TABLE. These have the value 0 in the attribute IS_ACCEPTED_NAME. Synonyms are loaded after all valid names have been loaded into TCl-Db, using the ADD_SP2K_SYNONYMS procedure. The procedure ADD_SP2K_VERNACULARS takes data from the SP2K_COMMON_NAMES_MV and SP2K_VALID_MV views and loads these data into the NAME, ASSERTION and VERNACULAR tables in TCl-Db.



```
SP2K_NAMEIDS_MV
CREATE MATERIALIZED VIEW
sp2k_nameids_mv
AS
SELECT a.name, a.record_id, b.name_id
FROM sp2k.taxa a, whouse.name b
WHERE a.name = b.name_text
```

```
SP2K_ONLY_MV
CREATE MATERIALIZED VIEW
sp2k_only_mv
AS SELECT t a.name, a.record_id, a.parent_id
FROM sp2k.taxa a LEFT OUTER JOIN whouse.name b
ON a.name = b.name_text
WHERE b.name_id is null
```

```
WHOUSE_SP2K_VALID_MV
CREATE MATERIALIZED VIEW
whouse_sp2k_valid_mv
AS
SELECT a.name_id, b.assertion_id, c.record_id
FROM whouse.name a, whouse.assertion b, sp2k.taxa_tree c
WHERE a.name_id = b.name_id
AND b.dbsource_id = c.record_id
AND b.source_id = 222
```

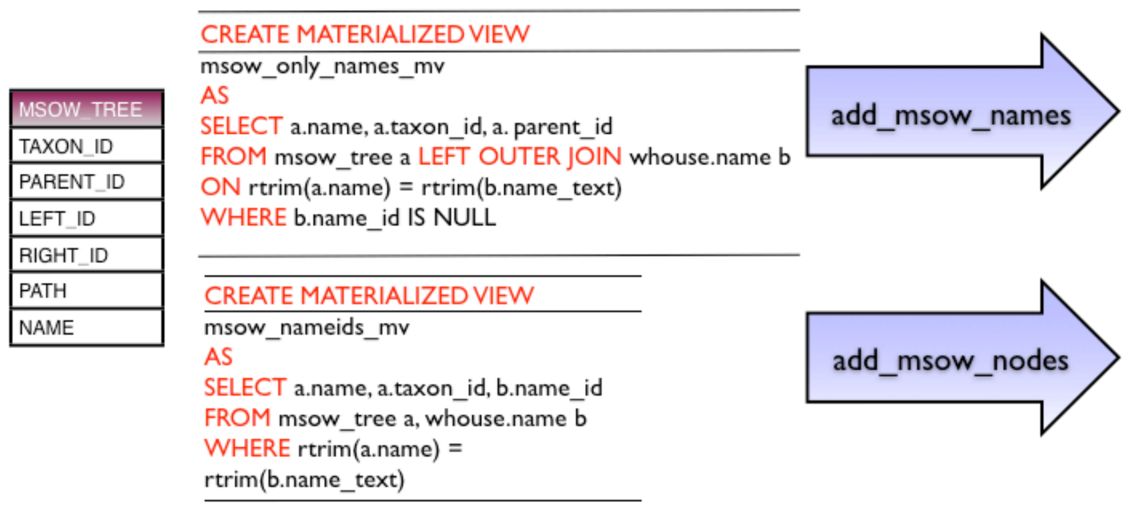
```
SP2K_COMMON_NAMES_MV
CREATE MATERIALIZED VIEW
sp2k_common_names_mv
AS
SELECT a.common_name, a.record_id, b.record_id valid_record_id
FROM common_names a, taxa b
WHERE a.name_code = b.name_code
AND b.is_accepted_name = 1
```

```
SP2K_SYNONYMS_MV
CREATE MATERIALIZED VIEW
sp2k_synonyms_mv
AS
SELECT record_id, name, taxon, parent_id
FROM taxa
WHERE is_accepted_name =0
AND parent_id in (
SELECTrecord_id
FROM taxa
WHERE is_accepted_name =1)
```

Figure 4.17: Overview of the Sp2000 data migration giving the tables, and views over these tables that are used in the PL/SQL procedures.

4.6 MSOW

The Mammal Species of the World (MSOW) is an online checklist from the Smithsonian National Museum of History. A plain text file was downloaded from the website http://nmnhgoph.si.edu/msw/ and the data were transformed into a simple table structure. This data structure represents, within a single table, the minimum data required for a data source, these are: a unique identifier, the name text and the hierarchical parent name text. The data needed to be given unique identifiers, which was done using an Oracle sequence [1], and parent-child relationships for the hierarchy were extracted from the download file. These data and the hierarchical data were then loaded into the table MSOW_TREE shown in Figure 4.18. Using this table, the unique MSOW names were collected into the materialized view MSOW_ONLY_NAME_MV and, for the names already in TCl-Db, the materialized view WHOUSE_NAMEIDS_MV pre-collected the data needed for loading into the ASSERTION table. Once these views are built, the procedures ADD_MSOW_NAMES and ADD_MSOW_NODES are then run.



```
CREATE MATERIALIZED VIEW
msow_only_names_mv
AS
SELECT a.name, a.taxon_id, a. parent_id
FROM msow_tree a LEFT OUTER JOIN whouse.name b
ON rtrim(a.name) = rtrim(b.name_text)
WHERE b.name_id IS NULL
```

```
CREATE MATERIALIZED VIEW
msow_nameids_mv
AS
SELECT a.name, a.taxon_id, b.name_id
FROM msow_tree a, whouse.name b
WHERE rtrim(a.name) =
rtrim(b.name_text)
```

Figure 4.18: Overview of the Mammal Species of the World data migration giving the tables and views used in the PL/SQL procedures ADD_MSOW_NAMES and ADD_MSOW_NODES

[1] A sequence is an object in Oracle that is used to generate a number sequence. These are useful when you need to create a unique number to act as a primary key.

4.6.1 Aves, early bird data

Additional data from a number of Aves checklists were made available to us through the Early Bird Project (Hackett, 2003). These data, summarised in Table 4.2, mostly came in the form of flat files. An extract of the data is given in Table 4.3. The data in these files were loaded into individual tables and transformed into the global schema. The transformation process included adding a NAME entry if the name did not already exist in the database, an ASSERTION entry to link the name to its original data source and a NODE entry for the classification data. PL/SQL procedures transformed the flat file structure shown in Table 4.3 into a hierarchical parent - child structure, e.g. *Parus* as a parent with *Parus montanus* as child. Using this transformed structure, we calculated nested sets and materialized paths for each node of the hierarchy, and produced the data, as sampled in Table 4.4. Additional data for rank and kingdom were extrapolated and added to the assertion rows. Some data cleaning was performed during transfer to the TCl-Db schema. This removed minor data inconsistencies in spelling of higher taxa names, duplicated values and inserted missing higher taxa values.

Check List	Total Names	Unique Names	TCl-Db Names
Morony, Bock and Farrand (247)	11396	659	10,796
Sibley and Monroe(248)	11,909	81	11,850
American Ornithological Union 83 (250)	2741	39	2716
American Ornithological Union 98 (251)	2914	60	2888
Peters (252)	11,218	1221	10,046
NAM980612 (253)	10,18	60	11,974
Bird_Names (256)	9652	101	9560
Clements (259)	9648	0	9657

Table 4.2: The transformation process produces a materialized view for each new name source, reconciling the names with those already within TCl-Db and identifying new names that need to be added. For each of the Aves checklists the number of names in each and the totals for new and existing TCl-Db names are given. The checklists are listed above in the order in which they were loaded into the TCl-Db schema.

```
ID Order Family Genus Species Name MBFnum SMnum
1 Tinamiformes Tinamidae Tinamus major Tinamus major 4 14
2 Tinamiformes Tinamidae Nothocercus bonapartei Nothocercus bonapartei 6 16
3 Tinamiformes Tinamidae Crypturellus soui Crypturellus soui 11 21
4 Tinamiformes Tinamidae Crypturellus cinnamomeus Crypturellus cinnamomeus 22 24
5 Tinamiformes Tinamidae Crypturellus boucardi Crypturellus boucardi 23 28
6 Tinamiformes Tinamidae Crypturellus kerriae Crypturellus kerriae 25 29
7 Gaviiformes Gaviidae Gavia stellata Gavia stellata 60 3845
8 Gaviiformes Gaviidae Gavia arctica Gavia arctica 61 3846
10 Gaviiformes Gaviidae Gavia immer Gavia immer 63 3848
11 Gaviiformes Gaviidae Gavia adamsii Gavia adamsii 64 3849
12 Podicipediformes Podicipedidae Tachybaptus dominicus Tachybaptus dominicus 71 3615
13 Podicipediformes Podicipedidae Podilymbus podiceps Podilymbus podiceps 72 3616
14 Podicipediformes Podicipedidae Podilymbus gigas Podilymbus gigas 73 3617
15 Podicipediformes Podicipedidae Podiceps auritus Podiceps auritus 77 3623
16 Podicipediformes Podicipedidae Podiceps grisegena Podiceps grisegena 78 3621
17 Podicipediformes Podicipedidae Podiceps nigricollis Podiceps nigricollis 80 3624
18 Podicipediformes Podicipedidae Aechmophorus occidentalis Aechmophorus occidentalis 84 3629
20 Procellariiformes Diomedeidae Diomedea exulans Diomedea exulans 86 3929
21 Procellariiformes Diomedeidae Diomedea albatrus Diomedea albatrus 89 3933
22 Procellariiformes Diomedeidae Diomedea nigripes Diomedea nigripes 90 3934
23 Procellariiformes Diomedeidae Diomedea immutabilis Diomedea immutabilis 91 3935
```

Table 4.3: Sample data from the Aves checklist flat files. This extract shows the first 23 lines of the file from American Ornithological Union 83. This flat file gives a numerical id, Order, Family, Genus and Species Names, followed by the corresponding identifier for the species in the checklists of Morony, Bock and Ferrand, and Sibley and Monroe.

NODE_ID	ASSERTION_ID	NAME_ID	SOURCE_ID	PATH	LEFT_ID	RIGHT_ID	PARENT_NAME_ID	TREE_ID
16660362	15337710	13234529	248	/14	2898	2993	13232598	280011
16660363	15337350	13232759	248	/13	2784	2897	13232598	280011
16660364	15339215	13236650	248	/12	2770	2783	13232598	280011
16660365	15338881	13236225	248	/11	1908	2769	13232598	280011
16660366	15339051	13236457	248	/10	1816	1907	13232598	280011
16660367	15338666	13235896	248	/9	1776	1815	13232598	280011
16660368	15339677	13237288	248	/8	404	1775	13232598	280011
16660369	15338459	13235592	248	/7	364	403	13232598	280011
16660370	15339223	13236660	248	/6	356	363	13232598	280011
16660371	15340407	13239850	248	/5	242	355	13232598	280011
16660372	15340551	13240465	248	/4	24	241	13232598	280011
16660373	15337191	15891304	248	/3	18	23	13232598	280011
16660374	15349053	14174735	248	/2	4	17	13232598	280011
16668411	15345647	13291365	248	/1	2	3	13232598	280011
16671318	15418688	13232598	248	/	1	23818	13232598	280011

Table 4.4: Sample data from Node table. Hierarchical queries can be performed on this transformed data set using 1. parent-child relationship presented in columns NAME_ID and PARENT_NAME_ID; 2. difference between LEFT_ID and RIGHT_ID columns presenting the nested set data and 3. using LIKE statements on the materialized paths presented in the column PATH.

4.7 Adding New Data Sources

Adding new data sources to TCl-Db is relatively easy, requiring only knowledge of SQL to build the tables for the new data source, and PL/SQL to copy the data in to the TCl-Db schema. The easiest route is to build a table structure that replicates the data source's flat file structure. This requires building a table for each file and loading the data directly into the table, using the SQLLDR utility. The process of mapping the tables and building the PL/SQL procedures is manual, though, once built, these can be called in triggers after INSERT, UPDATE and DELETE on the source tables. Database triggers are used to handle specific events on specific tables and they provide a significant benefit in data management (transferring data across schemas in this case). Triggers were implemented on the data source schemas to drive data transfer. When new data are added to the source tables, the trigger fires the relevant procedure. However, the source data structures have not so far proved to be stable and the triggers have been disabled. The data load steps are currently run manually in an effort to maintain and check the integrity of the data coming into the TCl-Db tables.

For each new data source, the classification data for the NODE table need to be built to enable the hierarchical queries. This requirement is not satisfied by some data providers, ITIS, GRIN and SP2K needed manual editing to remove disconnected nodes. Disconnected nodes occurred most often when a species or sub species name were labelled valid (or accepted) but the parent name was not considered valid. Only valid names were extracted for inclusion in the classification tree and, in some cases, the parent names were missed in the query. These were 'breaking' the tree and either the parent was identified manually and added to the tree data or the node had to be removed if a valid parent could not be identified. Finding these disconnected nodes is not a trivial task and was the most laborious step in the data load process. Another difficulty that was encountered was unique and persistent identification. In order to effectively use the GRIN, MSOW and the Early Bird data, unique identifiers had to be created for each datum entering the master table. Sp2000 was a problematic update, as it uses unique identifiers which are not persistent through releases. When adding the 2006 Sp2000 release we could not load just the new data. Instead we had to delete the older 2005 version and reload the newer version of Sp2000. Since the old Sp2000 identifiers no longer pointed to data at Sp2000, deleting the old version and replacing it with the new one seemed the most sensible option.

4.7.1 Data Availability

The data are available in two forms, Oracle EXP dumps and a MYSQL dump from a version ported to MySQL. The Oracle download consists of two EXP files, one full export which contains the full data warehouse including the source data silos, and the other is a simple export containing just the global schema and data. SQL scripts are also provided to replicate the table structures.

The MySQL download contains the global schema and data. An XML format of the integrated assertion data of the global schema is also available. These data can be downloaded from http://spira.zoology.gla.ac.uk/download.php along with full instructions on their use. The PL/SQL procedures and views used in the data loads are fully documented at http://spira.zoology.gla.ac.uk/doc.php.

4.8 Summary and Preview

This chapter described the implementation aspects of data integration undertaken in the course of constructing TCl-Db. Data loading, cleaning and structuring into trees was carried out using a mixture of software programs written in C++ and PL/SQL. Database view mechanisms and stored procedures played a decisive role in the success of this undertaking. Full details of imports from all the data sources were given. The next chapter will focus on how this data can now be used to satisfy user information needs.

Chapter 5

Database Utility and Web Tools

5.1 Overview

TCl-Db was primarily built to meet the requirements of the systematics/tree building community. This chapter exemplifies the utility of the database within two contexts: using the data in TCl-Db to translate search terms into those used in databases such as TreeBASE, and using TCl-Db for more complex analysis, to synonymise terms across various data sources. The first section details the queries that are supported by TCl-Db, with examples. We then go on to extend these queries and display the utility of the data warehouse in contributing to a better understanding of the individual data sources. Using a warehouse approach to meet the requirements has the added benefit of enabling queries that compare data sources side by side. Querying integrated data as a unit is a particular benefit of data warehouses. The final section details the web tools that were built to search the data in TCl-Db. Finally, we present a wrapper that uses the data in TCl-Db to deliver taxonomically intelligent queries on a local copy of TreeBASE.

5.2 Supported Queries

The most important requirement in the development of TCl-Db was to deliver taxonomically intelligent queries. These queries are: hierarchical queries, where the query term expands to include subordinate terms in the classification of choice, and the expansion of vernaculars and synonym queries to include valid names and other names associated with the original search term. The TCl-Db data model is described in Chapter 3, while the queries that this model and the implementation supports are exemplified here.

5.2.1 Hierarchical queries

The most important of the requirements was the capacity to store and query multiple classifications. Although a number of amalgamated database systems stored names from multiple sources, the classifications of those names were not stored. This was also deemed one of the most important features lacking in TreeBASE. TreeBASE contains taxon names but no classification. TCl-Db provides three mechanisms to query the hierarchical data: the Oracle Connect By query (Gennick, 2006), nested sets query and the materialised path query (Celko, 2004). These are outlined below.

Using Parent-Child Relationship on NODE

Simple queries can be performed using the parent-child relationship stored in the NODE table. For example, a very simple query can collect all species within a genus using the query shown in Appendix A (A1). An alternative form of this query is shown in A2 using rank data from the ASSERTION table.

Oracle's CONNECT BY statement

The CONNECT BY clause is an extension to SQL's SELECT query implemented within the Oracle RDBMS, specifically to enable hierarchical queries using parent rows and child rows. Within TCl-Db the CONNECT BY query also uses the parent-child relationship modelled by the attributes name_id and parent_name_id in the NODE table. For example, in Appendix A (A3) the CONNECT BY starts with Crocodilia and moves up the tree to the Root node. Queries A4 and A5 use an Oracle function SYS_CONNECT_BY_PATH which produces a delimited path listing of all names up to the root of the hierarchy.

Hierarchical queries using nested set, left and right IDs and paths

The nested set and path data have been included to make the system more accessible and portable to other database products, including MySQL. The nested set mechanism is described by Celko (2004) and these data need to be calculated using graph algorithms. The path string complements the nested mechanism. It turned out that although the nested set query as in

Appendix A (A6) is the fastest query when traversing down a tree, traversing up a tree is much harder with this method. Selecting the path string and iterating through this proved to be more efficient and is shown in A7. Query A7 is uses two queries. Since they can not be combined into a single query, the path has to be retrieved from the tables first, so that it can be used in a LIKE clause in the second query.

5.3 Data analysis Queries

The advantage of the data warehouse approach is that once data are replicated and transformed into a global schema, they can be queried as a unit. This is the most significant advantage of data warehousing, as certain complex queries can only be performed efficiently when the data are available in this way. The breadth of queries that are possible directly on the warehouse far exceeds any kind of interface that can be provided at individual sources. These queries are suited to the 'omics' style analyses which are prevalent in molecular biology and bioinformatics. The types of analyses on the data that are now possible are exemplified through some queries given here.

Initially, very simple comparisons were conducted between data sources. The overlap between ITIS and NCBI, using the query in Appendix A (A8), returns the number of overlapping names. The overlap was surprisingly low. From a total of 413,230 names in ITIS and 273,404 in NCBI only 48,355 names were common to both databases. Following on from this, we tried to identify distributional bias of the names within each kingdom in order to identify where the overlaps were and where the differences existed. While trying to quantify these differences we found that a comparison by kingdom did not form a simple query. This is because NCBI uses the Woese domain system of Bacteria, Archaea and Eukarya (Woese, 2004), while ITIS uses the Whittaker five kingdom system (Whittaker, 1959). Attempting to map these names was untenable. For example, it is difficult to equate Monera in ITIS to Bacteria and Archaea in NCBI. Also in NCBI the 'Fungi/Metazoa group' was too complex to map to Animalia in ITIS. This query highlights the fundamental differences in classification that many of the databases exhibit. A user querying NCBI with the term Monera may not get the expected results. The databases are quite different in their coverage of taxonomic data, prompting further questions. For example, the number of names unique to NCBI names that are species/subspecies and higher taxa names (Appendix A (A12)), is given in Figure 5.1 and Table 5.1 shows that there is significantly less overlap at the species level (13%) and lower ranks. These comparisons show

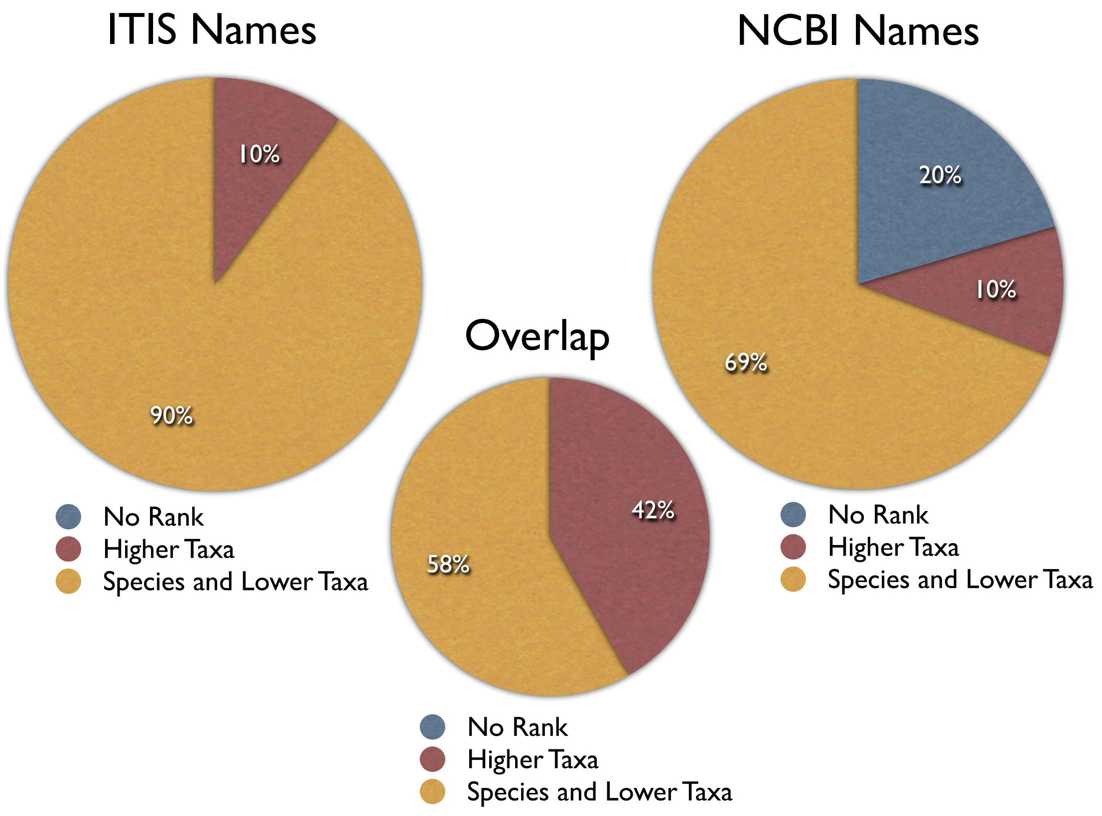


Figure 5.1: ITIS and NCBI comparison showing that the majority of names in both databases are species and lower taxa but the overlapping names are split almost equally between higher taxa and lower taxa ranks.

that the two databases are complimentary, and therefore have the potential of adding more value when used together. We are also able to use the integrated data to look at data coverage within groups. For example, given a genus we can count how many species and subspecies that genus contains across all the data sources.

One of the advantages of using a data warehouse is the ability to add to the existing data. The queries given in Appendix (A9 and A10) gather homonyms into a materialized view. Homonyms are names that are spelt in an identical manner but refer to different taxa. Such names arise mainly because the names of plants and animals are independent and there are no rules across the codes to forbid the use of a name already used in an other kingdom. A list of homonyms has been constructed and is available at `http://darwin.zoology.gla.ac.uk/~nanwar/animal_plant_dup_names.txt`. To simplify and avoid confusion during a search these

Rank	NCBI Count	ITIS Count	overlap with ITIS Count	%
Superkingdom	3	0	0	0
Kingdom	3	4	2	50
Subkingdom	0	2	0	0
superphylum	4	0	0	0
Phylum	81	69	55	79
Subphylum	14	17	12	70
Superclass	5	5	1	20
Class	203	156	114	73
Subclass	100	103	76	73
Superorder	49	41	31	75
Order	976	937	664	70
Suborder	325	437	189	43
Superfamily	593	286	153	53
Family	5204	6387	3581	58
Subfamily	1392	769	229	29
Genus	31,298	33,649	13,241	39
Subgenus	521	209	0	0
Species	171,156	189,497	25,804	13
Subspecies	4769	14358	349	2.5
Tribe	912	345	95	27
Subtribe	173	9	1	11
Varietas(Variety)	1268	9639	1	0.01

Table 5.1: Summary of ITIS and NCBI content categorised by rank. The overlap, with respect to ITIS, is given in the final column.

names are tagged with their respective kingdoms in parentheses, for example, search results for the query term Morus are shown in Figure 5.2. Homonyms in higher taxa can also cause significant problems for hierarchical queries using the Oracle CONNECT BY statement. In ITIS, for example, there is a loop in the tree at the name_id 13102529 for the name Mastigophora, since this taxa is both a valid genus in the kingdom Plantae and a valid sub phylum in the kingdom Animalia. Identifying these homonyms enables these data to be tagged in such a way that many of the problems and confusion they cause can be overcome.

Data quality is of particular interest, and queries in TCl-Db enable data to be compared side by side making differences and discrepancies more obvious. Data quality and data integrity queries can check the names across databases to identify, for example, misspellings in names. In TCl-Db misspelt names can be identified by gathering all names unique to one data source and then comparing these to the names in the rest of the database, while allowing for mismatches. This was done for the class Aves. An initial comparison identified that ITIS had more names in this class, so for data quality we looked first at those names in NCBI that were not in ITIS. The

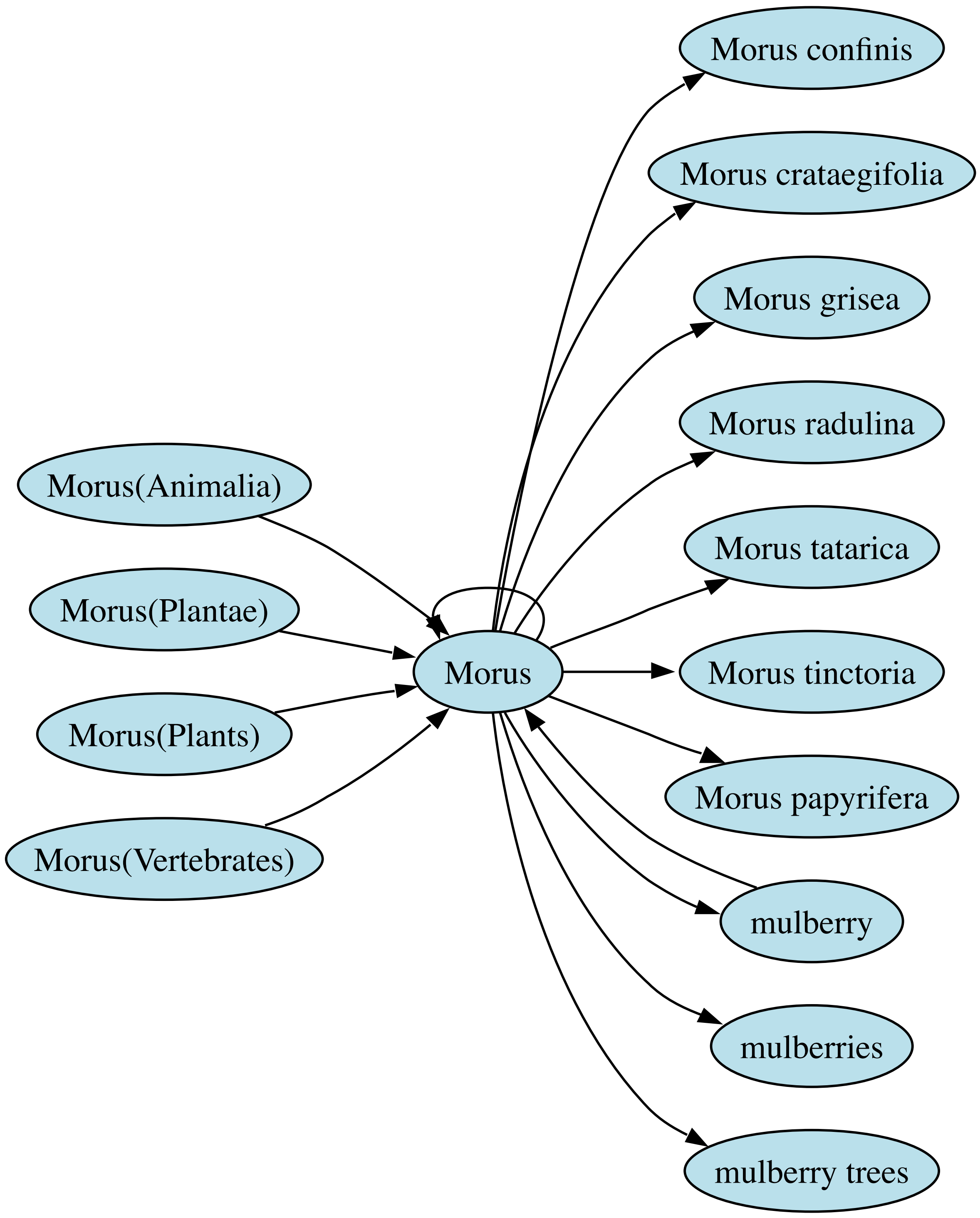


Figure 5.2: Query results for the search term Morus. Since Morus is a homonym the name with the kingdom in parentheses has been added so that users can easily see the term exists validly in two kingdoms.

unique NCBI Aves subset was extracted and a script iterated through each name using Agrep (Wu & Manber, 1992) to compare it to all other names in TCl-Db. Agrep is a text searching tool that allows strings to be compared while allowing for mismatches, i.e. errors. This analysis is described in Chapter 6.

TCl-Db can also be used to look at the content of particular databases. For example, we are able to count the number of the bacterial species names in NCBI that are trinomial rather than binomial. The query in Appendix A (A13) uses the LIKE condition in the where clause to find names that have the pattern '% % %' i.e. any string followed by a space, followed by any string and a space followed by any string. Simple queries like this can be used to get a better understanding of data quality and to determine where in the warehouse constraints and rules can be placed. For example, it would be inappropriate to add an integrity rule to the warehouse restricting species names to binomials. This is an example of a data integrity query. While performing these queries we also found numerous examples of names like "genus sp." in NCBI. Usually these names are attached to sequences for organisms that have sequence data, the organism though has only been identified into a genus with no specific name assigned. Also, many taxa in NCBI have simply been named as an "environmental sample".
Although it would be inappropriate to modify the source data entering TCl-Db, the examples above show that the data can be tagged with metadata once they are identified. Data integrity differs from data quality in that integrity refers to the validity of data in terms of consistency and data quality refers to the correctness of data in terms of accuracy. In TCl-Db the data sources are assumed to be correct. There are cases, however, where correct data entered into a database with no checks and no referential integrity can result in multiple entries, i.e., poor data integrity. For example, we identified three assertions for the name Mastigophora (TCl-Db name_id 13102529). This is because in ITIS this name has three valid entries. Not only is this a homonym, but within the Plant Kingdom it has two valid entries at the rank genus with Taxon Serial Numbers (TSN) 14271 and 14272. See `http://www.itis.usda.gov/servlet/SingleRpt/SingleRpt?search_topic=TSN&search_value=14271` and `http://www.itis.usda.gov/servlet/SingleRpt/SingleRpt?search_topic=TSN&search_value=14272`. These data integrity issues in the source databases can be identified more easily in TCl-Db. They can be found with an SQL statement as in query A10 in Appendix A, which identifies duplicate names into a materialised view. Each of the entries in the view were checked individually to determine which were homonyms and which were duplicate entries within the same kingdom. Some of those identified from this view are listed at

http://spira.zoology.gla.ac.uk/itis_valid_dups.txt. A similar example of poor data integrity in one of the source databases, SP2K, can be shown in the records for Vertebrata (record_id 2348763), Amphibia (record_id 2349507) and Isoptera (record_id 2348853) which are all in the kingdom Animalia. In one version of SP2K these are not accepted names and they point to the valid name Rhodomelaceae (record_id 1248761). These records are incorrect because the valid name Rhodomelaceae is in the plant kingdom and not the animal kingdom. The query A11 in Appendix A is used to identify and link names via synonyms and vernaculars across the databases, answering the question "how many names in the synonym_name table are also considered to be valid names". Such names could have entered the synonym_name table because at least one data source considers the name a synonym. Using several similar SQL queries, we found that not only do NCBI and ITIS differ in their coverage of names but names that do overlap may also be treated differently. For example, 866 ITIS valid names are considered to be synonyms in NCBI.

All linked names, misspellings, homonyms and data recovered from these queries have been placed into the table: name_search which can be searched using the example query A14 in Appendix A. The result returned from this query is shown in Figure 5.2.

5.3.1 Comparing classifications.

Comparing classifications is a complex problem that is more easily accomplished through graph based queries (Zhong *et al.*, 1996, 1999) than the set based queries within SQL. The importance of mapping taxonomies to each other is demonstrated with queries such as gathering data from one system using the classification of another. It could be, for example, that a user wishes to retrieve all sequence data for "Metazoa". Another example is highlighted by the case of "Ecdysozoa". The Ecdysozoa are a group of protostome animals which include the Arthropoda and Nematoda, and several smaller phyla (Aguinaldo *et al.*, 1997). Proponents of this clade may wish to use it as a search term, but currently the NCBI taxonomy does not include this term. To gather sequence data for this group requires mapping the term on to the NCBI classification.

A direct comparison of NCBI nodes and ITIS nodes from query A15 in Appendix A gives 44,320 names common to both classifications. Extending this query (A16) we can tell how many of these do not have the same parent name and are potentially classified differently. Queries to map across classifications are also possible using TCl-Db. Using hierarchical queries it is possible, for example, to take children of specific nodes in one classification and compare them to the children nodes in another classification. Discrepancies can be identified for those children

CHILD	PARENT_NCBI	PARENT_ITIS
Crocodylidae	Archosauria	Crocodilia
Tomistoma	Gavialinae	Crocodylidae
Osteolaemus	Crocodylinae	Crocodylidae
Crocodylus	Crocodylinae	Crocodylidae

Table 5.2: Child nodes of the term Crocodylidae that are in both NCBI and ITIS but classified differently. These are the results from query A17, Appendix A.

whose parent names are different. An example is given in query A17 which finds the child nodes for the term Crocodylidae (given in Figure 3.1) for NCBI and ITIS; the classifications overlap but are not the same. By creating a set of the child nodes in NCBI and a set of the child nodes in ITIS, we can identify from these sets which children overlap but do not share the same parent. The two classifications in this case are completely different and do not merge until the genera and species. ITIS does not recognise the name Crocodylinae, the parent of *Crocodylus* in NCBI.

The remainder of this chapter outlines the individual web tools created to perform query expansion using TCl-Db. In the final section, the web tools are brought together in one application, that enables taxon queries through TreeBASE .

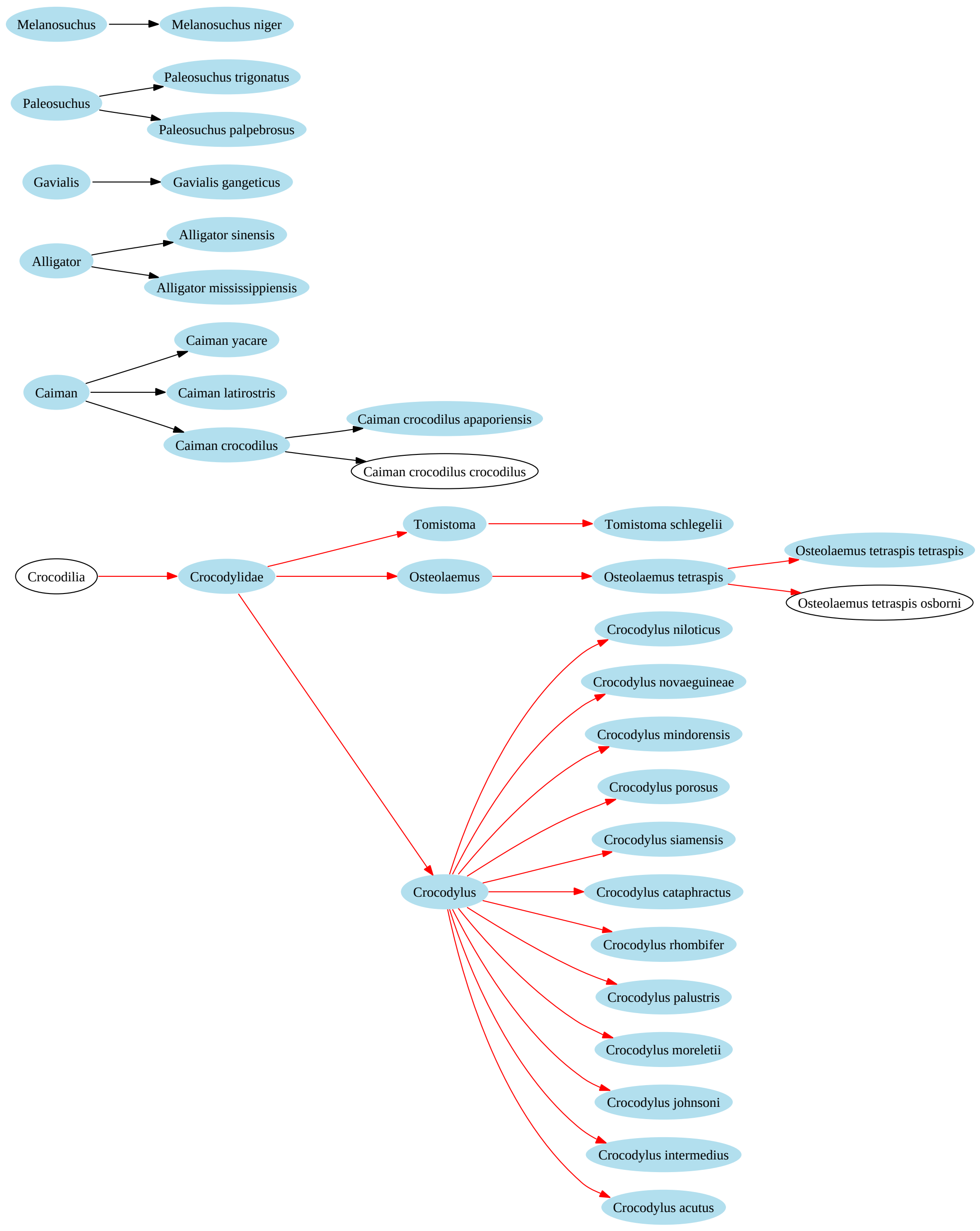


Figure 5.3: Crocodylidae Query: NCBI and ITIS. The NCBI classification is given in Figure 3.1. The ITIS classification of the family Crocodylidae is highlighted with the red edges NCBI classification in black. All common names across the two classifications are highlighted in blue. The classifications were merged using an SQL query. The query takes all nodes in the NCBI classification and uses these nodes to gather the same nodes within the ITIS classification. The diagram was created using webdot, e.g. `http://spira.zoology.gla.ac.uk/ClassificationWebdot.php?name_id=13232588&tree_id=1` for ITIS and `http://spira.zoology.gla.ac.uk/ClassificationWebdot.php?name_id=13232588&tree_id=2` for NCBI.

5.4 TCl-Db Web Tools

Taxon names are keys to biological data (Geoffroy, 2001), and in this capacity they are commonly used as search terms to retrieve data in many systems. TCl-Db warehouse was developed primarily to aid information retrieval from TreeBASE, through taxon names. This section describes web based search tools that utilise the TCl-Db integrated data, and a TreeBASE wrapper using a local copy of TreeBASE whose taxon names have been mapped to TCl-Db. Query terms given in the wrapper are transformed into taxon queries which are then performed on the mapped TreeBASE taxa in TCl-Db. We first describe the generic tools that may be used to browse, visualise and search for names stored within TCl-Db.

All the applications described here are located on the TCl-Db web page at `spira.zoology.gla.ac.uk`. The tools are built using PHP, PHP Hypertext Processor programming language (Zend Technologies, 2006), JavaScript, CSS, and the XMLHttpRequest Object is used to populate parts of the interface (Darie & Brinzarea, 2006). PHP is a very easy to use scripting language that makes development of web interfaces from databases such as MySQL and Oracle quick and cost effective. PHP is used primarily to access the data in the databases through the Oracle Call Interface (OCI) functions for Oracle. Alongside the traditional web interface for TCl-Db, there are web services providing a service oriented architecture to enable interoperability with other systems. These were also built using PHP, through re-using code already developed and PHP's web service development tools for XML-RPC (XML- Remote Procedure Call) (Winer *et al.*, 1999) and SOAP (Simple Object Access Protocol) (Gudgin *et al.*, 2003).

5.4.1 TCl-Db Search Tool

This section describes the scripts that were built to query and visualise data in TCl-Db. These tools can be used to link TCl-Db to other systems that need to support taxonomically intelligent queries.

Using scientific names as search terms is complicated by the fact that taxon names are in Latin and are often difficult to spell. This can be overcome using string matching technologies (Alberga, 1967; Navarro, 2001; Pfeifer *et al.*, 1995, 1996). By using these tools, the system can provide 'a catch' on each query: if no data are found for the query given, then alternatives are suggested to the user. Taxon names also change from time to time and data linked to an older usage, a synonym, may not be retrieved when another name takes common use. Linked names within TCl-Db can be used to expand search terms to include both synonyms and vernaculars.

One other feature of taxon names that should be considered by a system that allows taxon names as search terms, is that taxon names are also contained within a hierarchy. In many cases the search term given is not a simple search and the user expects the query to expand hierarchically. These requirements are fulfilled by a search tool for TCl-Db.

The search service can be found at the URL http://spira.zoology.gla.ac.uk/search_tcl.php. The interface requires the user to submit a search term. The search terms are first checked against the names in the TCl-Db table NAME_SEARCH for an exact match. This table contains all linked names, therefore, the search term can be a synonym, vernacular, higher taxon name or valid species name. If no hits are returned, the query is then rechecked against the database using Agrep (Wu & Manber, 1992). The Agrep results are refined, based on the query length using the Levenshtein (Cohen *et al.*, 2003) method.

On returning either an exact match, or providing links to approximate matches, the returned result, including linked names, is shown diagrammatically and in a drop down menu (Figure 5.4). The user can select from the drop down list the name for which he wishes to view the assertion data. The assertion data are name data from each of the data sources included within TCl-Db. The detailed view for the term Casuariidae, shown in Figure 5.5, gives the databases that contain the name, the synonym details, vernacular details and links to the original data sources. These are termed the assertion data. The data given for valid names in the columns above are: the search term, data source of the term, the data source identifier, rank, kingdom, the parent of the term in that data source hierarchy and a link to the children of that term. Synonyms and vernaculars show the same data, except for the rank and hierarchy data. The assertion data show repeated values for NCBI and ITIS, which is due to the way data are loaded. Although names are stored only once, the assertions of that name (i.e. which data source that name came from) can have multiple values if there is more than one copy of that data source. Both ITIS and NCBI have been updated and show two and three assertions, respectively, for the name Casuariidae. Should this result set become too verbose, it can be condensed by adding a distinct clause to the SQL query in the PHP script. The data include the direct parent in the hierarchy and a link to browse the immediate children within the original source hierarchy. The details for any synonyms and vernaculars are also listed in this view.

In addition to the simple search page, a second interface is provided to browse through particular classifications. This page can be accessed from the search page by clicking on the Browse button or directly from the URL http://spira.zoology.gla.ac.uk/browse/tcl_browse.php. The user is presented with a choice of three check boxes, and selecting any of them starts the

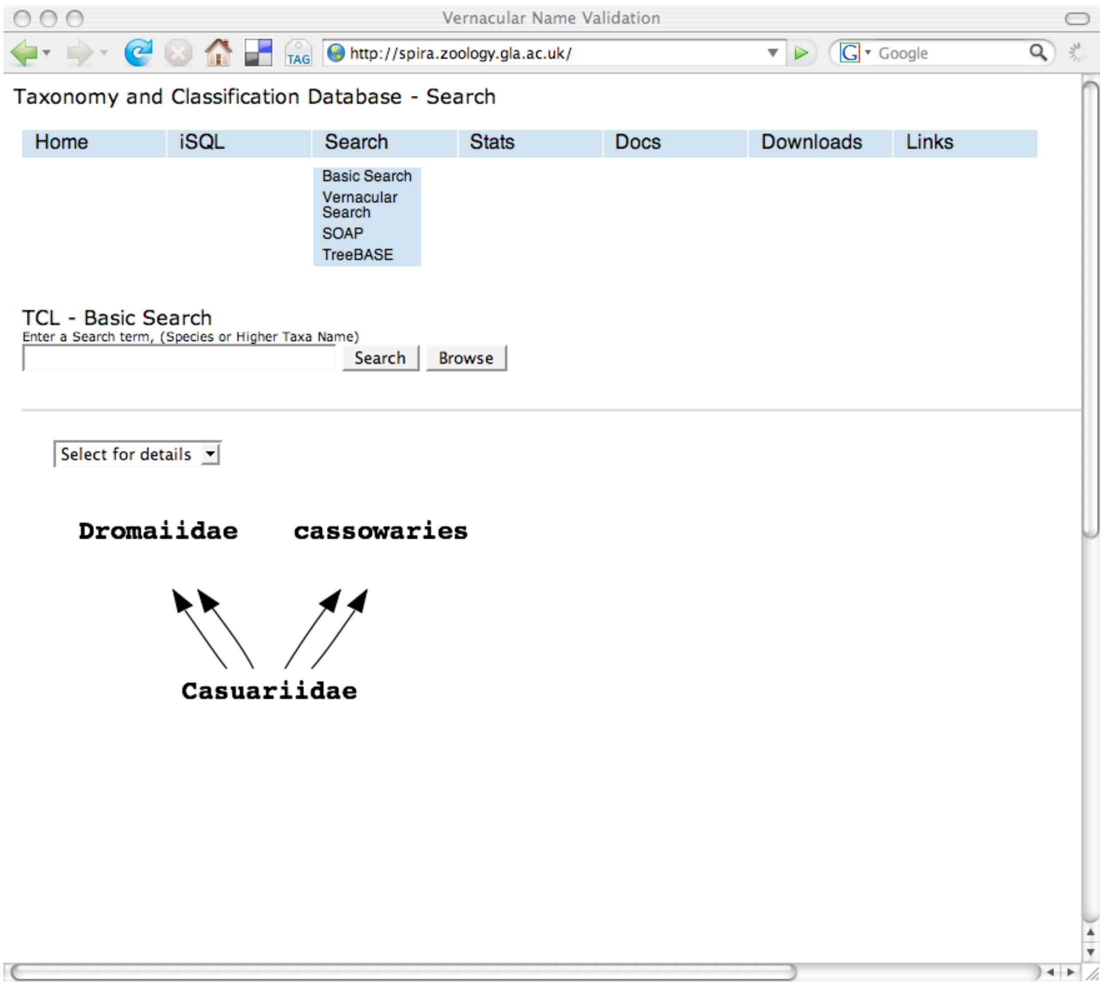
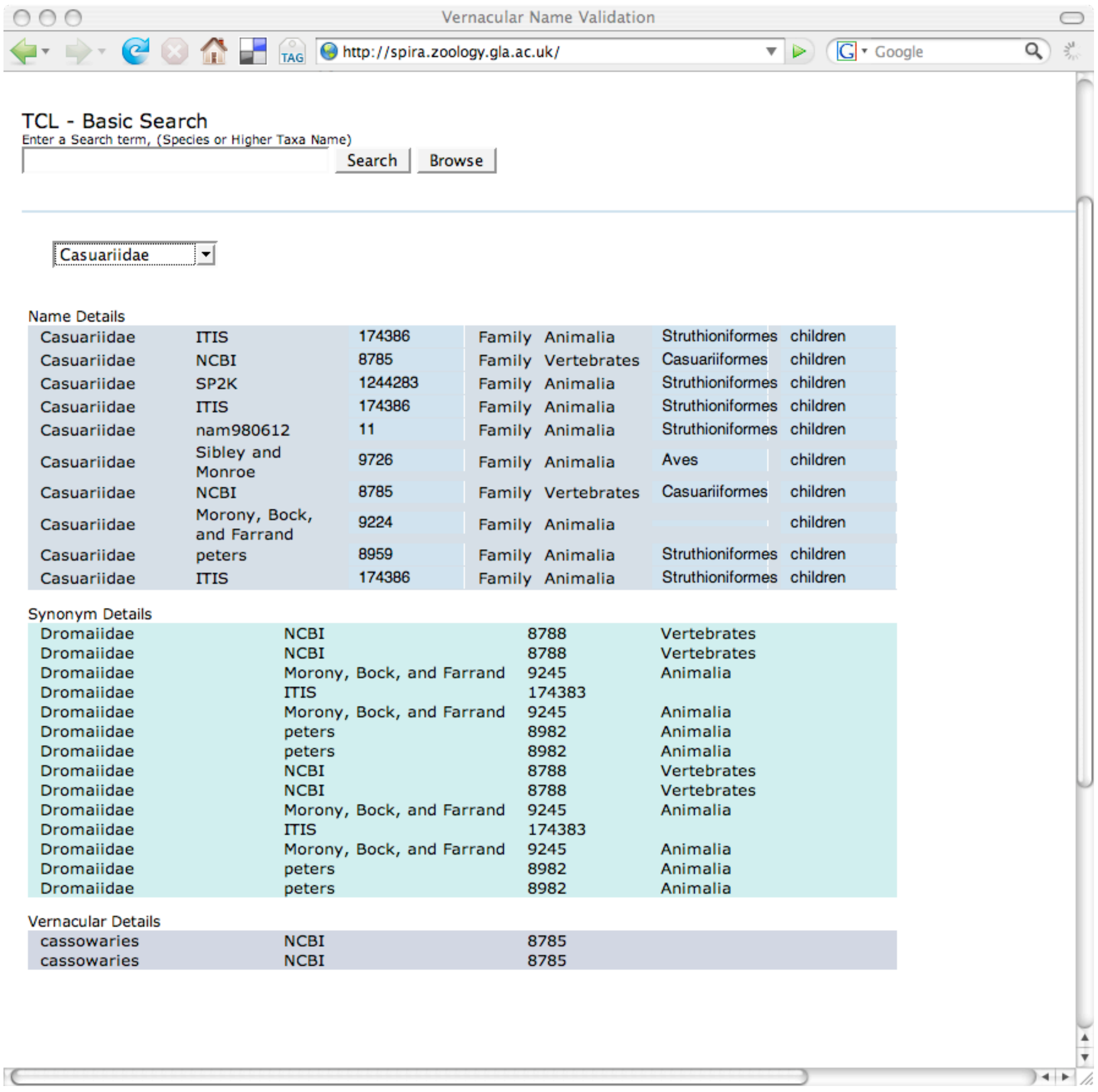


Figure 5.4: Search for the term Casuariidae presents users with a mapping to the synonym Dromaiidae. Mappings are also presented in a diagram. The diagram shows which names are linked. If a name is linked to itself it usually represents the valid name. There are two arrows linking the term Casuariidae, which represents the fact that these links were made through two data sources. If there is only one arrow, then only one data source made the link.



TCL - Basic Search

Enter a Search term, (Species or Higher Taxa Name)

Search Browse

Casuariidae

Name Details

Casuariidae	ITIS	174386	Family	Animalia	Struthioniformes	children
Casuariidae	NCBI	8785	Family	Vertebrates	Casuariiformes	children
Casuariidae	SP2K	1244283	Family	Animalia	Struthioniformes	children
Casuariidae	ITIS	174386	Family	Animalia	Struthioniformes	children
Casuariidae	nam980612	11	Family	Animalia	Struthioniformes	children
Casuariidae	Sibley and Monroe	9726	Family	Animalia	Aves	children
Casuariidae	NCBI	8785	Family	Vertebrates	Casuariiformes	children
Casuariidae	Morony, Bock, and Farrand	9224	Family	Animalia		children
Casuariidae	peters	8959	Family	Animalia	Struthioniformes	children
Casuariidae	ITIS	174386	Family	Animalia	Struthioniformes	children

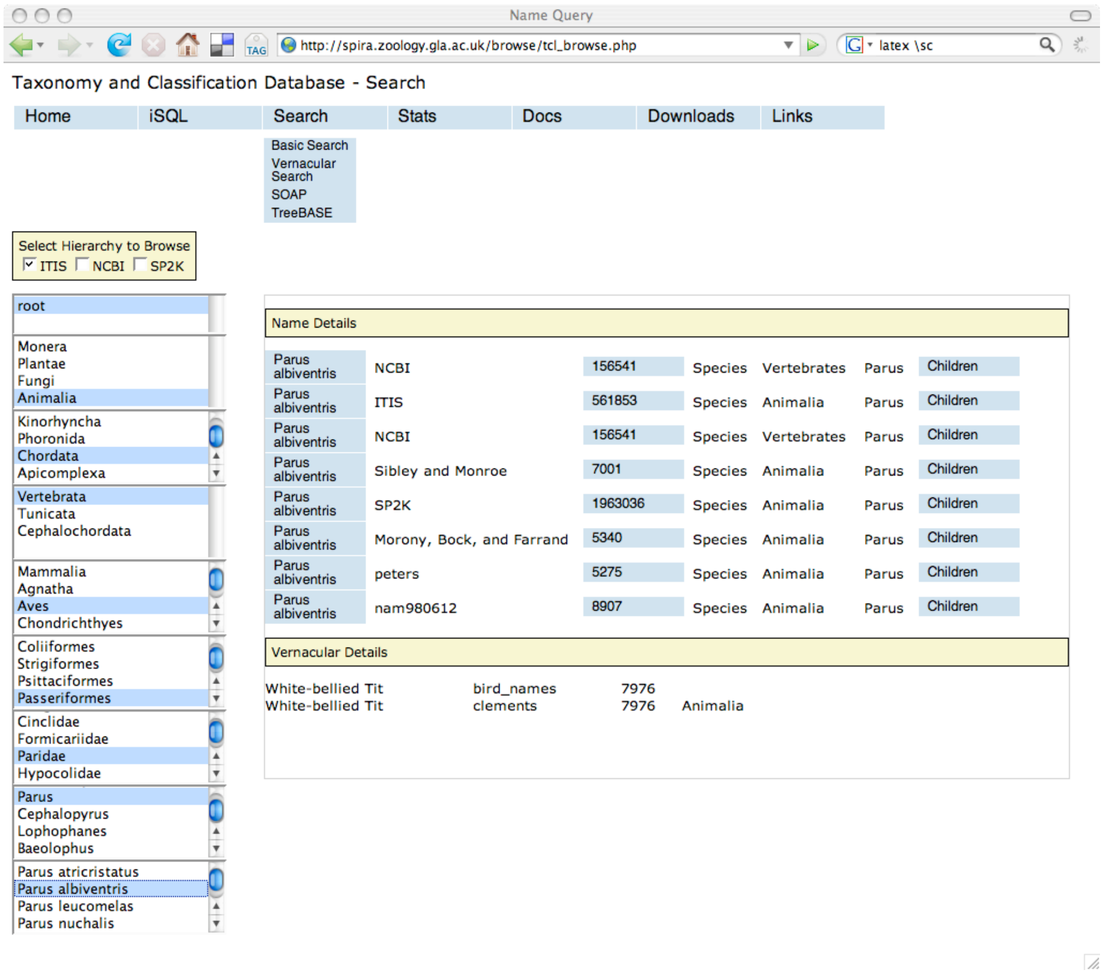
Synonym Details

Dromaiidae	NCBI	8788	Vertebrates
Dromaiidae	NCBI	8788	Vertebrates
Dromaiidae	Morony, Bock, and Farrand	9245	Animalia
Dromaiidae	ITIS	174383	
Dromaiidae	Morony, Bock, and Farrand	9245	Animalia
Dromaiidae	peters	8982	Animalia
Dromaiidae	peters	8982	Animalia
Dromaiidae	NCBI	8788	Vertebrates
Dromaiidae	NCBI	8788	Vertebrates
Dromaiidae	Morony, Bock, and Farrand	9245	Animalia
Dromaiidae	ITIS	174383	
Dromaiidae	Morony, Bock, and Farrand	9245	Animalia
Dromaiidae	peters	8982	Animalia
Dromaiidae	peters	8982	Animalia

Vernacular Details

cassowaries	NCBI	8785
cassowaries	NCBI	8785

Figure 5.5: The detailed view for the term Casuariidae.



Taxonomy and Classification Database - Search

Select Hierarchy to Browse: [✓ ITIS] NCBI SP2K

root

Monera
Plantae
Fungi
Animalia

Kinorhyncha
Phoronida
Chordata
Apicomplexa

Vertebrata
Tunicata
Cephalochordata

Mammalia
Agnatha
Aves
Chondrichthyes

Coliiformes
Strigiformes
Psittaciformes
Passeriformes

Cinclidae
Formicariidae
Paridae
Hypocolidae

Parus
Cephalopyrus
Lophophanes
Baeolophus

Parus atricristatus
Parus albiventris
Parus leucomelas
Parus nuchalis

Name Details

Parus albiventris	NCBI	156541	Species	Vertebrates	Parus	Children
Parus albiventris	ITIS	561853	Species	Animalia	Parus	Children
Parus albiventris	NCBI	156541	Species	Vertebrates	Parus	Children
Parus albiventris	Sibley and Monroe	7001	Species	Animalia	Parus	Children
Parus albiventris	SP2K	1963036	Species	Animalia	Parus	Children
Parus albiventris	Morony, Bock, and Farrand	5340	Species	Animalia	Parus	Children
Parus albiventris	peters	5275	Species	Animalia	Parus	Children
Parus albiventris	nam980612	8907	Species	Animalia	Parus	Children

Vernacular Details

White-bellied Tit	bird_names	7976	
White-bellied Tit	clements	7976	Animalia

Figure 5.6: The Classification Browse Interface allows the user to click through the classification.

search. Once selected, the next series of select boxes appears, and the user clicks through the boxes for the classification path of interest. A double click on a name will display assertion data.

5.4.2 Visualisation Tools: Linked Names and Classifications with Webdot

The Dot command line programme and language (Koutsoos *et al.*, 1996) draws directed graphs, Webdot (Ellson, 2006) is a CGI program that converts the dot graphs into an image that can be included into a webpage. Webdot images are used to display linked names produced by TCl-Db as shown in Figure 5.4 and also Figure 5.15, and are particularly useful for displaying portions of the classifications (Figure 5.16). The Webdot application was installed to run locally. It takes as input a dot file, (an example dot file is shown below in Table 5.3). This file produces the image shown in Figure 5.15.

```
digraph G
{
graph [size="16,2"];
"Morus"->"Morus";
"Morus"->"Morus confinis";
"Morus"->"Morus crataegifolia";
"Morus"->"Morus grisea";
"Morus"->"Morus radulina";
"Morus"->"Morus tatarica";
"Morus"->"Morus tinctoria";
"Morus"->"Morus papyrifera";
"Morus"->"mulberry";
"Morus"->"mulberries";
"Morus"->"mulberry trees";
"Morus(Animalia)"->"Morus";
"Morus(Plantae)"->"Morus";
"Morus(Plants)"->"Morus";
"Morus(Vertebrates)"->"Morus";
"mulberry"->"Morus";
}
```

Table 5.3: Example dot file used Webdot to produce the image in Figure 5.16

The PHP functions within the TCl-Db basic search produce a dot file for each search. The webdot CGI then converts this file into the images (Figure 5.4 and Figure 5.15). These views were very useful in the understanding of the integrated data. A further standalone tool was developed to display the full hierarchy below a search term. The application, shown in Figure 5.7, returns the full classification below the term Crocodylidae for the classification tree from ITIS. A search form version is provided at http://spira.zoology.gla.ac.uk/classificationwebdotallnodes.php. However, for larger queries, with more than 30 nodes the graphs become difficult to read and hence the interface is only useful for smaller subtrees.

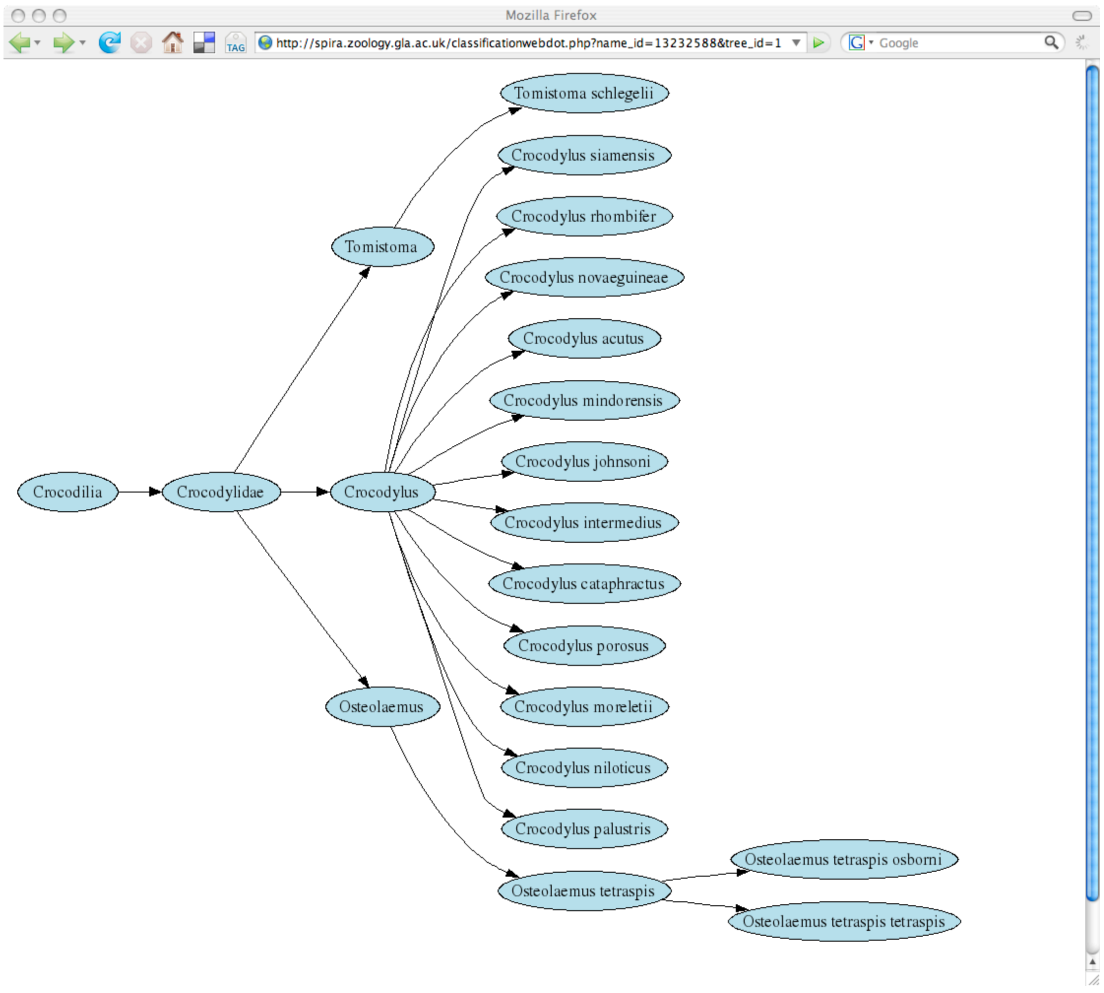


Figure 5.7: Interface: Classification displayed in Webdot for Crocodylidae. From URL http://spira.zoology.gla.ac.uk/classificationwebdot.php?name_id=13232588&tree_id=1

5.4.3 Supporting vernacular search terms

Vernacular names are commonly used as search terms (see analysis of TreeBASE search data in Chapter 7). Although spiders, fruit fly, or birds are more familiar terms, they do not convey the same meaning as their Latin counterparts Archanae, *Drosophila melanogaster*, or Aves. Scientific names are more specific in their meaning than vernacular names. Vernacular names are often used because they are not specific and have broader scope and are therefore used as general or loose queries. Most databases primarily deliver scientific names and vernaculars may or may not be given. This is because vernaculars are not included within the scope of the database if they are not needed. There seems to be poor link up between valid scientific names and vernacular names. With the current tools, it is a cumbersome task for a biologist to translate a list of vernacular names into scientific names. TCl-Db can be used to map vernacular names to valid names, and the application described here exemplifies how TCl-Db can be used to simplify or semi-automate data collection using vernacular names. For example, such an application can be used to collect sequence data for several organisms, using vernaculars as query terms. Links to NCBI have been included in the application as an example. The common names can be searched using approximate spelling, or a phonetic spelling with suggestions returned for the user to select from. Given the awkward spelling of many names, a secondary search page provides suggestions as the user types, which may be more useful to some users. The URL for the vernacular search form is `http://spira.zoology.gla.ac.uk/app`.

When using a vernacular term, most users know roughly what they are looking for, i.e. they use a "they will know it when they see it" search. These queries usually start with an initial non-specific or "broad" query term in the expectation of returning a large set of names which they can then browse through to find the Latin name of interest. In this capacity, the vernacular search term is a kind of "loose" query. The looseness of vernaculars makes the term relatively stable, for example, the term birds translates to the scientific name Aves. Taxonomists may revise what the term Aves means phylogenetically, however, the details of that change (inclusion or exclusion of several species) does not change the general definition of the vernacular term, i.e., egg-laying vertebrates characterised primarily by feathers, forelimbs modified as wings, and hollow bones, etc.

For users seeking to collect sequence data, the NCBI web site enables them to conduct a vernacular search, and many other taxonomic data sources also provide a vernacular search tool. However, most systems with this capability fall short for a number of reasons. The search interfaces enable only a single name search at a time. A user with a list of names has to search each name separately and then collate his data. In a system that does translate the vernacular term, it does so only on the valid term and the term is not expanded further, i.e. hierarchically. To use the birds example again, this would translate to Aves but it is likely that the user requires the species names within Aves and not the actual term itself. As we have already shown, there is also the issue of taxonomic coverage within individual databases, and amalgamated databases such as TCl-Db provide far more coverage.

The interface uses PHP and javaScript (Darie & Brinzarea, 2006). There are three separate PHP scripts. The first gives the initial search page (Figure 5.8) and is found at the URL http://spira.zoology.gla.ac.uk/app. On this page, users can copy and paste a list of vernacular names into the text box, while an alternative search page provides users with suggestions as they type. The suggestions interface is based on the Google suggests (http://www.google.com/webhp?complete=1&hl=en).

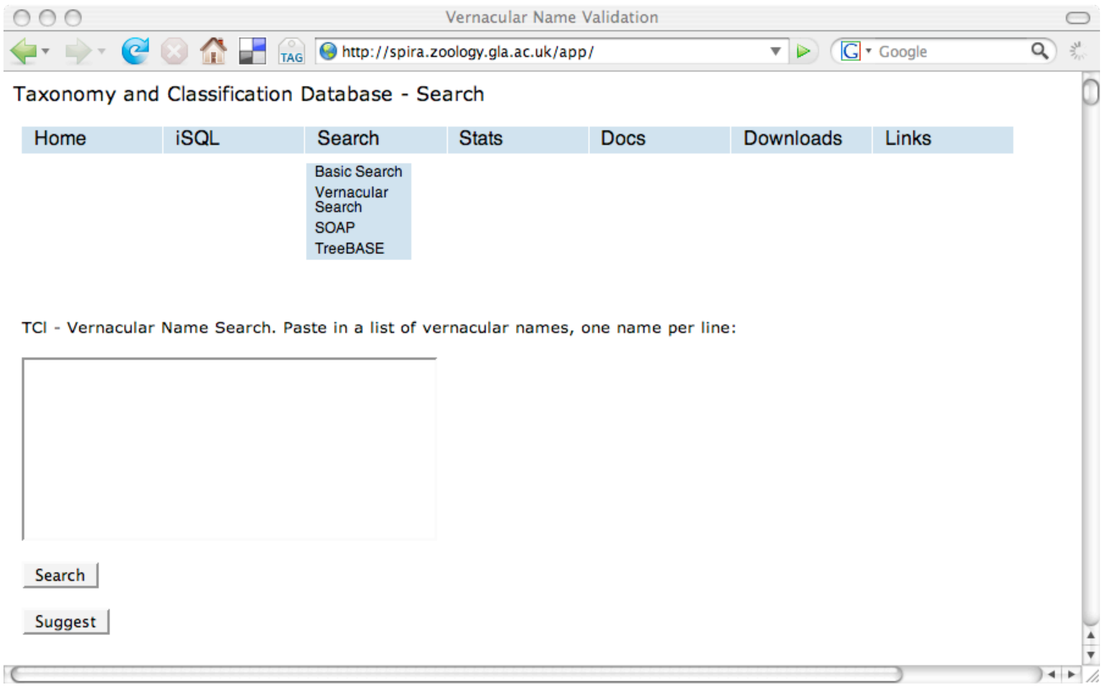
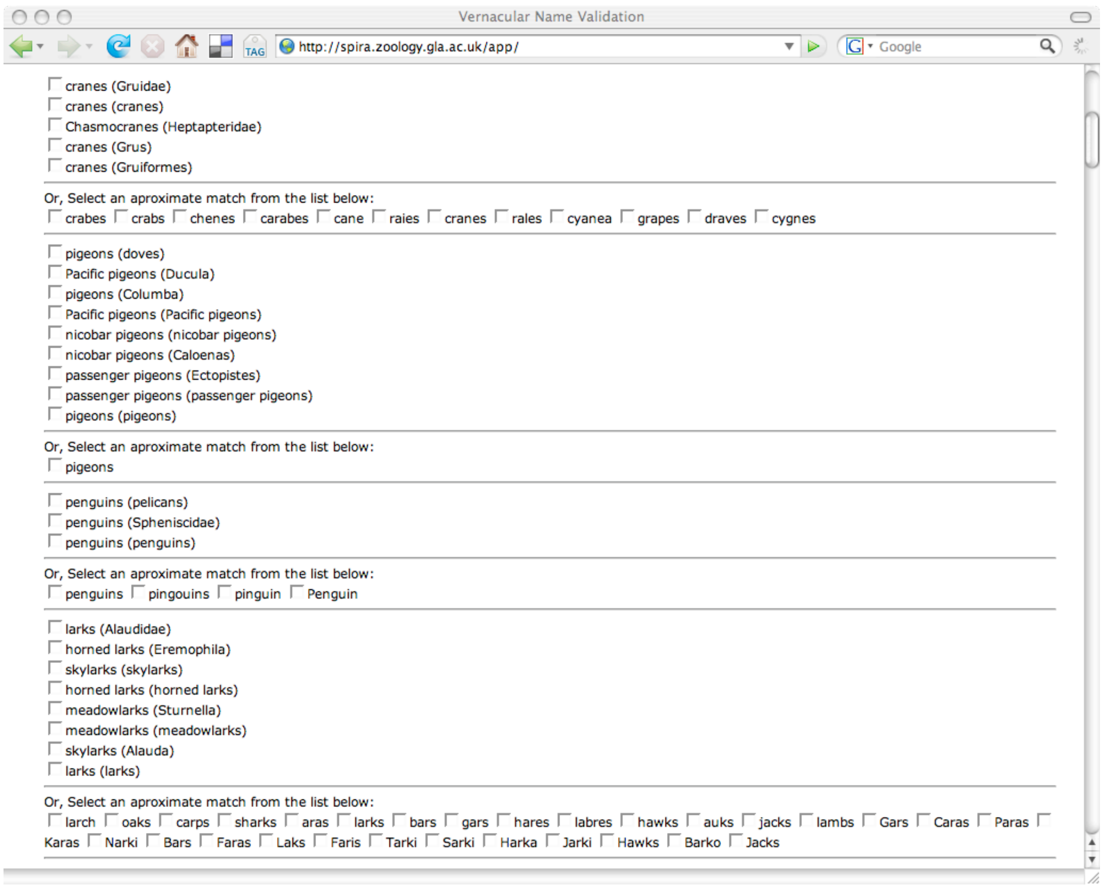

Vernacular Name Validation
http://spira.zoology.gla.ac.uk/app/
Google
Taxonomy and Classification Database - Search
Home
iSQL
Search
Stats
Docs
Downloads
Links
Basic Search
Vernacular Search
SOAP
TreeBASE
TCl - Vernacular Name Search. Paste in a list of vernacular names, one name per line:
Search
Suggest

Figure 5.8: Vernacular Query form at http://spira.zoology.gla.ac.uk/app

The script uses a list of names which were dumped into a text file from a TCl-Db table holding mapped names. The script takes the search terms given and searches each through the text file of TCl-Db names using Agrep, in order to find initial matches. With a mismatch of two agrep returns a very large list of matches. The use of Agrep with a mismatch of two is a bit of a compromise, as the effect of increasing the mismatch returns even more data when the search term is short and reducing it to one misses too many potential matches when the search term is longer. This is analogous to the precision and recall measures used in information retrieval, as good recall returns as many relevant matches as possible while minimising the number of non-relevant matches (Singhal, 2001). The matches returned from Agrep are refined using the length of the query term and the Levenshtein method (Cohen *et al.*, 2003). From these results, suggestions for taxon names that match the query are returned to the user in a second query form. This second script builds a form from which users select the names of interest returned from the initial query. Further suggestions are also made to users to help them find what they are looking for, see Figure 5.9. After selecting the terms of interest using the check boxes and clicking on the next button, the following page (and final script) displays the selections with a drop down menu from which the user can view assertion data (Figure 5.10).


Vernacular Name Validation
http://spira.zoology.gla.ac.uk/app/
Google

☐ cranes (Gruidae)
☐ cranes (cranes)
☐ Chasmocranes (Heptapteridae)
☐ cranes (Grus)
☐ cranes (Gruiformes)

Or, Select an aproximate match from the list below:
☐ crabes ☐ crabs ☐ chenes ☐ carabes ☐ cane ☐ raies ☐ cranes ☐ rales ☐ cyanea ☐ grapes ☐ draves ☐ cygnes

☐ pigeons (doves)
☐ Pacific pigeons (Ducula)
☐ pigeons (Columba)
☐ Pacific pigeons (Pacific pigeons)
☐ nicobar pigeons (nicobar pigeons)
☐ nicobar pigeons (Caloenas)
☐ passenger pigeons (Ectopistes)
☐ passenger pigeons (passenger pigeons)
☐ pigeons (pigeons)

Or, Select an aproximate match from the list below:
☐ pigeons

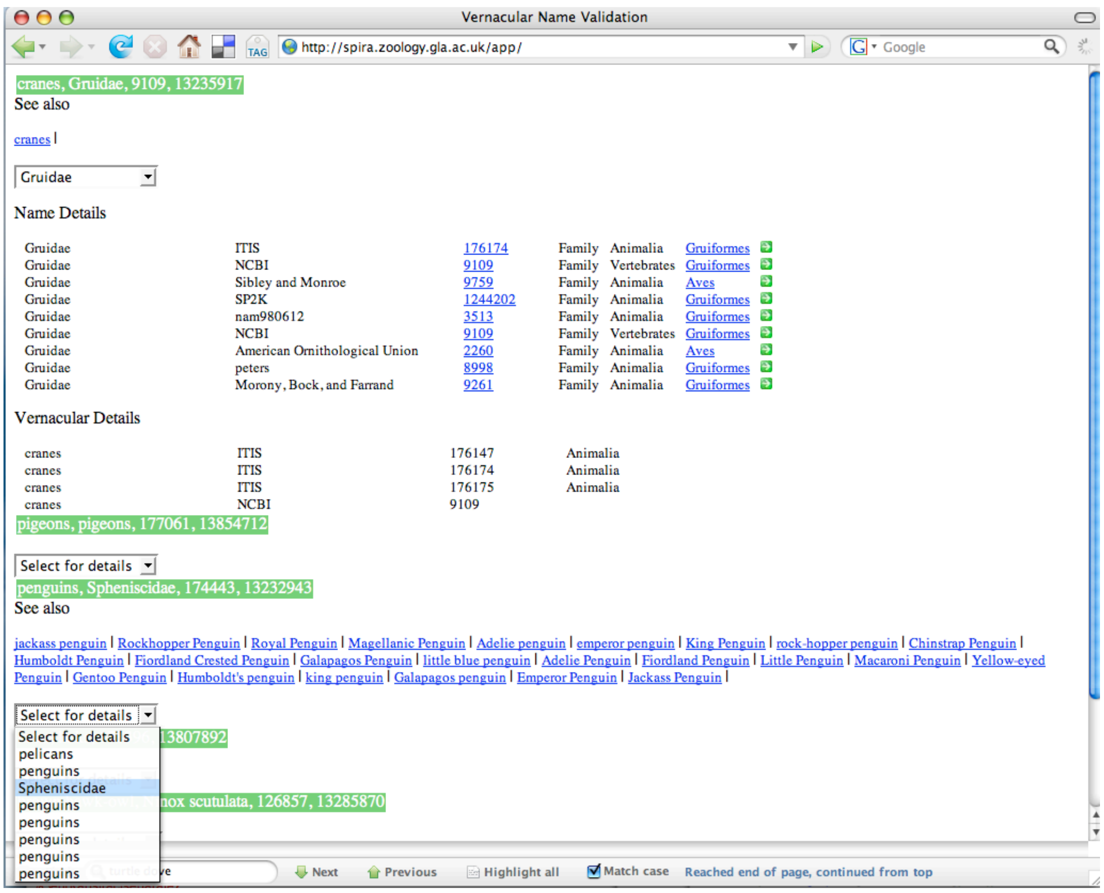
☐ penguins (pelicans)
☐ penguins (Spheniscidae)
☐ penguins (penguins)

Or, Select an aproximate match from the list below:
☐ penguins ☐ pingouins ☐ pinguin ☐ Penguin

☐ larks (Alaudidae)
☐ horned larks (Eremophila)
☐ skylarks (skylarks)
☐ horned larks (horned larks)
☐ meadowlarks (Sturnella)
☐ meadowlarks (meadowlarks)
☐ skylarks (Alauda)
☐ larks (larks)

Or, Select an aproximate match from the list below:
☐ larch ☐ oaks ☐ carps ☐ sharks ☐ aras ☐ larks ☐ bars ☐ gars ☐ hares ☐ labres ☐ hawks ☐ auks ☐ jacks ☐ lambs ☐ Gars ☐ Caras ☐ Paras ☐ Karas ☐ Narki ☐ Bars ☐ Faras ☐ Laks ☐ Faris ☐ Tarki ☐ Sarki ☐ Harka ☐ Jarki ☐ Hawks ☐ Barko ☐ Jacks

Figure 5.9: Screen shot of Vernacular Query Results from a query on cranes, pigeons, penguins, larks at http://spira.zoology.gla.ac.uk/app



Vernacular Name Validation

http://spira.zoology.gla.ac.uk/app/

cranes, Gruidae, 9109, 13235917
See also

cranes |

Gruidae

Name Details

Gruidae	ITIS	176174	Family	Animalia	Gruiformes	🟩
Gruidae	NCBI	9109	Family	Vertebrates	Gruiformes	🟩
Gruidae	Sibley and Monroe	9759	Family	Animalia	Aves	🟩
Gruidae	SP2K	1244202	Family	Animalia	Gruiformes	🟩
Gruidae	nam980612	3513	Family	Animalia	Gruiformes	🟩
Gruidae	NCBI	9109	Family	Vertebrates	Gruiformes	🟩
Gruidae	American Ornithological Union	2260	Family	Animalia	Aves	🟩
Gruidae	peters	8998	Family	Animalia	Gruiformes	🟩
Gruidae	Morony, Bock, and Farrand	9261	Family	Animalia	Gruiformes	🟩

Vernacular Details

cranes	ITIS	176147	Animalia
cranes	ITIS	176174	Animalia
cranes	ITIS	176175	Animalia
cranes	NCBI	9109	

pigeons, pigeons, 177061, 13854712

Select for details

penguins, Spheniscidae, 174443, 13232943
See also

jackass penguin | Rockhopper Penguin | Royal Penguin | Magellanic Penguin | Adelie penguin | emperor penguin | King Penguin | rock-hopper penguin | Chinstrap Penguin | Humboldt Penguin | Fiordland Crested Penguin | Galapagos Penguin | little blue penguin | Adelie Penguin | Fiordland Penguin | Little Penguin | Macaroni Penguin | Yellow-eyed Penguin | Gentoo Penguin | Humboldt's penguin | king penguin | Galapagos penguin | Emperor Penguin | Jackass Penguin |

Select for details

Select for details
pelicans
penguins
Spheniscidae
penguins
penguins
penguins
penguins
penguins

13807892

nox scutulata, 126857, 13285870

Figure 5.10: Screen shot of Vernacular Query Results - Data page

5.4.4 A TreeBASE Wrapper

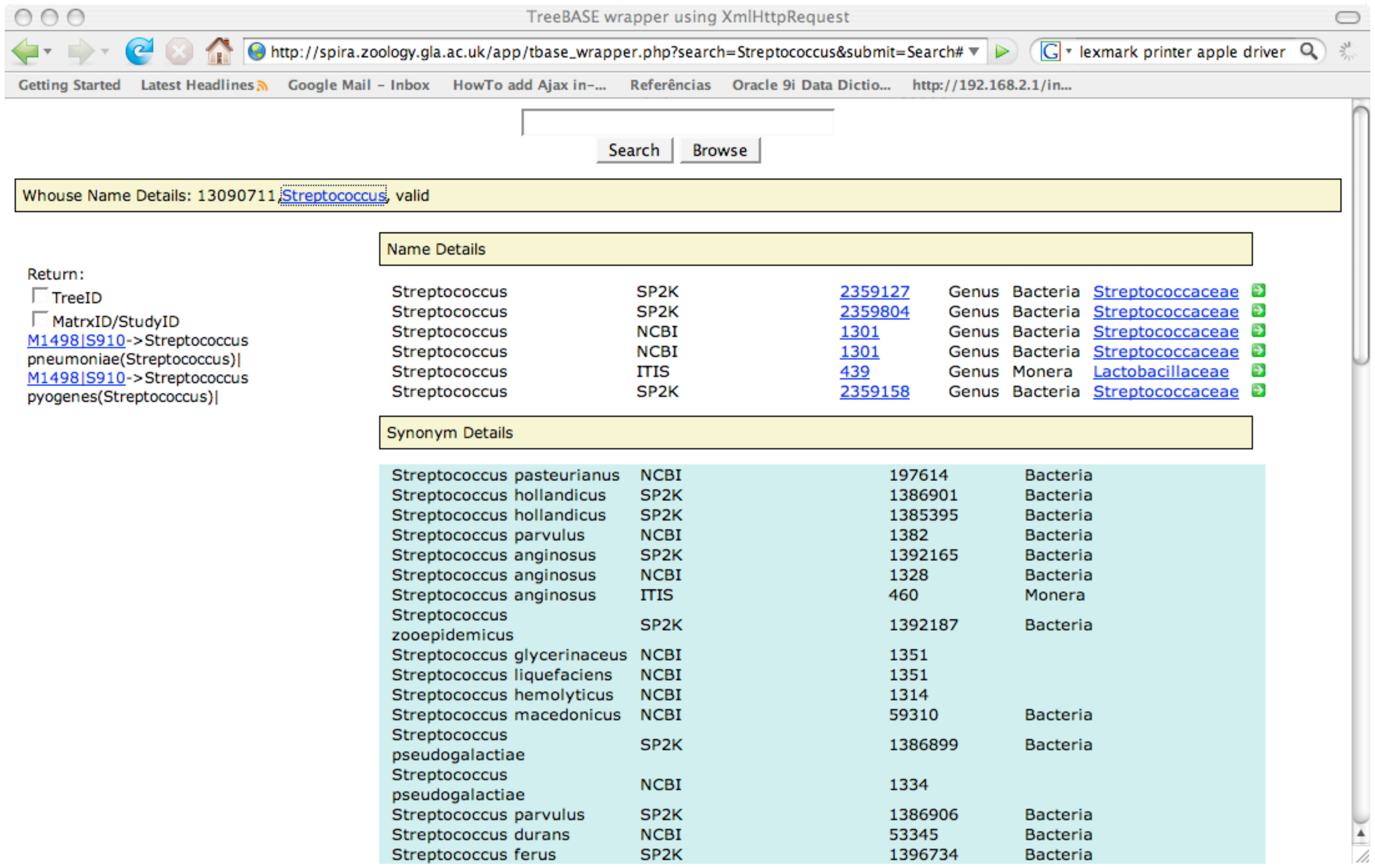
Taxonomic Requirements of TreeBASE

TreeBASE (Morell, 1996) contains phylogenies for more than 90,000 taxa. Despite the intrinsic taxonomic content, at design, the developers of TreeBASE purposely excluded taxonomy (Morell, 1996). The TreeBASE interface (www.treebase.org) supports six query types: author, citation, study accession number, matrix accession number, taxon and structure. The taxon search, however, does not perform adequately. This search option does not effectively support higher taxa queries or synonym and vernacular queries.

From a biologists perspective, the taxon search option does not return the expected results. The query term "Aves" currently returns 5 studies however, there are many more studies containing Aves (birds) within TreeBASE. Higher taxa terms such as Aves are not being expanded to include the scientific names contained within them. Queries performed on TreeBASE return only data where the search term matches exactly a term contained in the study. Similarly a vernacular query such as "birds", returns no data because it is not contained in any study. The synonyms also fail to return complete result sets. The taxonomic content and structure of TreeBASE does not support these queries, as query terms are not expanded to include associated terms and as a result incomplete results are returned. TCl-Db was built to improve the current data retrieval options within TreeBASE.

The taxonomic queries that TreeBASE should support were stated in the introduction, query terms should expand hierarchically and vernacular and synonym queries should be supported through the provision of query expansion to linked valid names. TCl-Db was designed to provide a taxonomic infrastructure to TreeBASE and supports these queries.

We have built a simple web application that enables taxon queries via TCl-Db to return the relevant TreeBASE data. The interface provides both a search form (Figure 5.11) and a classification browse form (Figure 5.12) which returns either TreeBASE TREEID's or STUDYID's. These link to the current online TreeBASE interface via hyperlinks. Unfortunately, the copy of TreeBASE that this application is built on is over two years old. However, the application code uses data in materialized views which query the TreeBASE TAXA and TCl-DB NAMES tables and the views are set to automatically refresh when new data are loaded into these parent tables. Therefore, on update of the TreeBASE schema, the application code will require no significant changes. The two materialized views used by the application (Query 1 and Query 2, are shown in Figure 5.13) make use of the taxon mappings table TREEBASE_WHOUSE_MAPPED.


TreeBASE wrapper using XmlHttpRequest
http://spira.zoology.gla.ac.uk/app/tbase_wrapper.php?search=Streptococcus&submit=Search#
lexmark printer apple driver
Getting Started
Latest Headlines
Google Mail - Inbox
HowTo add Ajax in-...
Referências
Oracle 9i Data Dictio...
http://192.168.2.1/in...
Search
Browse

Whouse Name Details: 13090711 Streptococcus, valid

Return:
☐ TreeID
☐ MatrxID/StudyID
M1498|S910->Streptococcus pneumoniae(Streptococcus)|
M1498|S910->Streptococcus pyogenes(Streptococcus)|

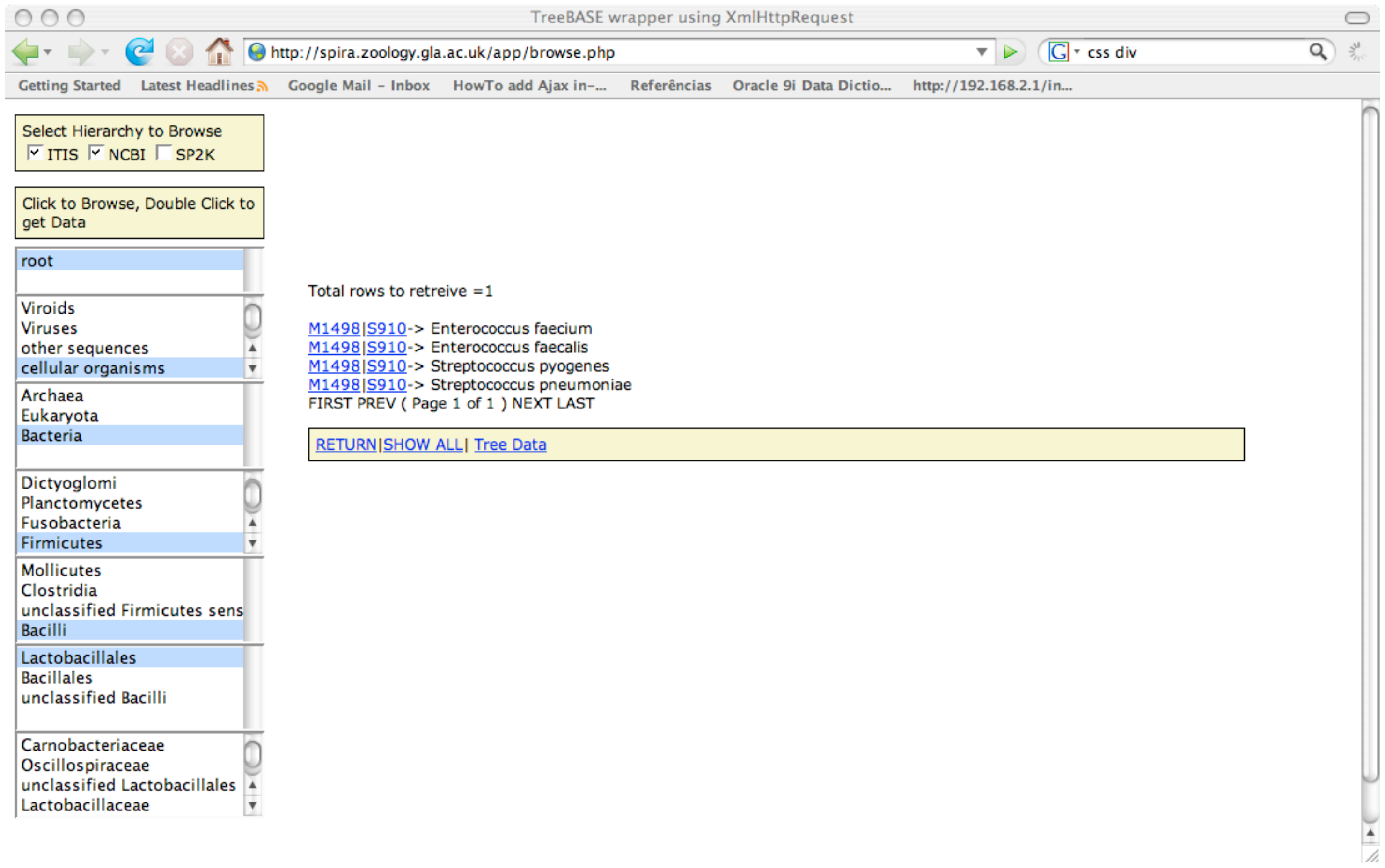
Name Details

Streptococcus	SP2K	2359127	Genus	Bacteria	Streptococcaceae	➡
Streptococcus	SP2K	2359804	Genus	Bacteria	Streptococcaceae	➡
Streptococcus	NCBI	1301	Genus	Bacteria	Streptococcaceae	➡
Streptococcus	NCBI	1301	Genus	Bacteria	Streptococcaceae	➡
Streptococcus	ITIS	439	Genus	Monera	Lactobacillaceae	➡
Streptococcus	SP2K	2359158	Genus	Bacteria	Streptococcaceae	➡

Synonym Details

Streptococcus pasteurianus	NCBI	197614	Bacteria
Streptococcus hollandicus	SP2K	1386901	Bacteria
Streptococcus hollandicus	SP2K	1385395	Bacteria
Streptococcus parvulus	NCBI	1382	Bacteria
Streptococcus anginosus	SP2K	1392165	Bacteria
Streptococcus anginosus	NCBI	1328	Bacteria
Streptococcus anginosus	ITIS	460	Monera
Streptococcus zooepidemicus	SP2K	1392187	Bacteria
Streptococcus glycerinaceus	NCBI	1351	
Streptococcus liquefaciens	NCBI	1351	
Streptococcus hemolyticus	NCBI	1314	
Streptococcus macedonicus	NCBI	59310	Bacteria
Streptococcus pseudogalactiae	SP2K	1386899	Bacteria
Streptococcus pseudogalactiae	NCBI	1334	
Streptococcus parvulus	SP2K	1386906	Bacteria
Streptococcus durans	NCBI	53345	Bacteria
Streptococcus ferus	SP2K	1396734	Bacteria

Figure 5.11: TreeBase Wrapper Screen shot - Search Page



Select Hierarchy to Browse
[✓ ITIS] [✓ NCBI] SP2K

Click to Browse, Double Click to get Data

root

Viroids
Viruses
other sequences
cellular organisms

Archaea
Eukaryota
Bacteria

Dictyoglomi
Planctomycetes
Fusobacteria
Firmicutes

Mollicutes
Clostridia
unclassified Firmicutes sens
Bacilli

Lactobacillales
Bacillales
unclassified Bacilli

Carnobacteriaceae
Oscillospiraceae
unclassified Lactobacillales
Lactobacillaceae

Total rows to retreive =1

M1498|S910-> Enterococcus faecium
M1498|S910-> Enterococcus faecalis
M1498|S910-> Streptococcus pyogenes
M1498|S910-> Streptococcus pneumoniae
FIRST PREV (Page 1 of 1) NEXT LAST

RETURN|SHOW ALL| Tree Data

Figure 5.12: TreeBase Wrapper Screen shot - Browse Page

The data in this table are from a combination of exact and approximate text matching on the taxonname field in the TreeBASE TAXA table and the TCl-Db NAME table. The exact matching (case insensitive) was a simple SQL query. A Perl script ran the approximate queries and loaded the data into a separate table. After some manual editing, these two tables were combined to give the master table TREEBASE_WHOUSE_MAPPED used by the materialized views shown in Figure 5.13.

Query 1. TREEBASE_WHOUSE_NODE_MATRIX

```
CREATE MATERIALIZED VIEW treebase_whouse_node_matrix
REFRESH FAST ON COMMIT
AS
(SELECT a.matrixid, b.studyid, b.taxonid, b.name_id,
c.parent_name_id, c.tree_id, c.right_id, c.left_id
FROM treebase.matrix a, treebase.treebase_whouse_mapped b,
whouse.node c, treebase_matrixtaxa d
WHERE b.taxonid = d.taxonid
AND a.matrixid = d.matrixid
AND b.name_id = c.name_id)
```

Query2. TREEBASE_WHOUSE_TREETAXA

```
CREATE MATERIALIZED VIEW treebase_whouse_treetaxa
REFRESH FAST ON COMMIT
AS
(SELECT a.taxonid, b.name_id, b.treeid
FROM treebase.treebase_whouse_mapped a, treebase.treetaxa b
WHERE a.taxonid = b.taxonid)
```

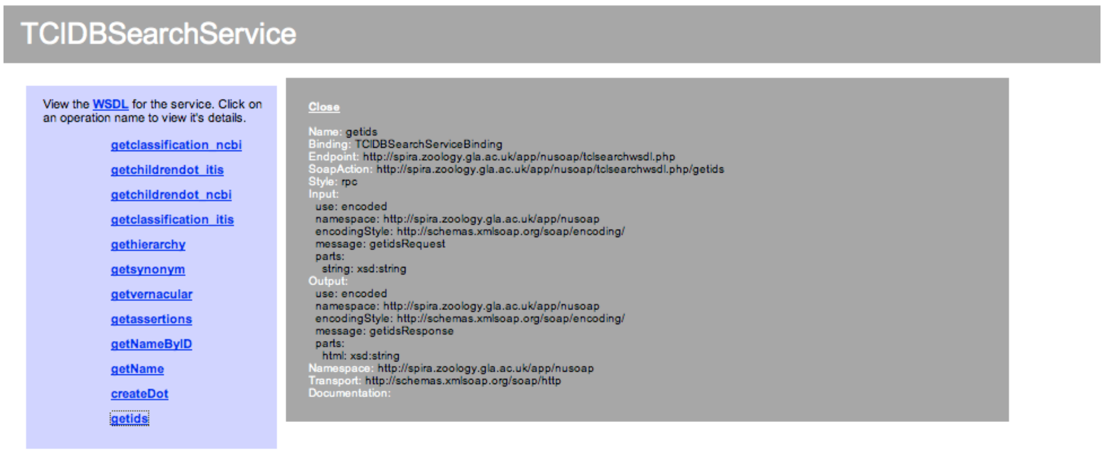
Figure 5.13: TreeBase Wrapper Materialized Views

The data in the views are accessed via PHP and JavaScript. A query using a vernacular term in the search form will return a list of linked taxon names from which the user can select TreeBASE data. For example, the search term “Song Sparrow” returns *Melospiza melodia*. The search form also enables the user to use an approximate spelling, for example, the search term "Caenorabditis" returns no data but suggests "Caenorhabditis" as a search. The browse form allows the users to first select which hierarchy they wish to browse, the choices given are ITIS, NCBI and Sp2000, and then select the taxon for which they want to get TreeBASE data. The application can be accessed from the URL http://spira.zoology.gla.ac.uk/app/tbase_wrapper.php.

5.4.5 SOAP Tools

Introduction

Most systems, and even sometimes the underlying tools within those systems, are built in isolation and rarely work together seamlessly. It is quite rare to find an all encompassing monolithic tool that contains every application or algorithm that a users wants to use. More often, tools are developed in isolation and then built into a system. What this means for users is that they often have to wait for useful algorithms and tools to become available in the applications they use, or they have to use these tools in the native forms and transform the inputs and outputs as required. For example, a task performed by many molecular biologists through web tools takes a sequence of interest from NCBI (www.ncbi.nlm.nih.gov) to conduct a BLAST search, the results from the BLAST search are manually examined, and the user selects the relevant hits. These are gathered into FASTA format and then aligned using ClustalW (www.ebi.ac.uk/clustalw/). This is a very simple example of a workflow which can be performed from several resources on the web. There has been a huge investment in the development of automatic workflows to seamlessly manage the transfer of data and results from one application to the next (Hoon *et al.*, 2003; Shannon *et al.*, 2006), in the example above from BLAST to ClustalW. This kind of application integration can be performed in the traditional manner using a common API (Application Programming interface). In this way the applications can be strung together with relative ease. Just as data are integrated into larger systems to ease interoperability, applications and tools are integrated for the same purpose (Jepsen, 2001). Solutions for providing the same seamless interoperability over the web have come to be known as "Web services" (Ferris, 2003; Jepsen, 2001). These services are based on various XML technologies: UDDI (Universal Description, Discovery and Integration) which enables services to be discovered; WSDL (Web Services Definition Language) (Chinnici *et al.*, 2004) which is used to describe the syntax of web services; and SOAP (Simple Object Access Protocol) which is a message syntax for sending and receiving XML messages within Web services. SOAP is


TCIDBSearchService

View the WSDL for the service. Click on an operation name to view it's details.

```
Name: getids
Binding: TCIDBSearchServiceBinding
Endpoint: http://spira.zoology.gla.ac.uk/app/nusoap/tclsearchwsdl.php
SoapAction: http://spira.zoology.gla.ac.uk/app/nusoap/tclsearchwsdl.php/getids
Style: rpc
Input:
  use: encoded
  namespace: http://spira.zoology.gla.ac.uk/app/nusoap
  encodingStyle: http://schemas.xmlsoap.org/soap/encoding/
  message: getidsRequest
  parts:
   string: xsd:string
Output:
  use: encoded
  namespace: http://spira.zoology.gla.ac.uk/app/nusoap
  encodingStyle: http://schemas.xmlsoap.org/soap/encoding/
  message: getidsResponse
  parts:
   html: xsd:string
Namespace: http://spira.zoology.gla.ac.uk/app/nusoap
Transport: http://schemas.xmlsoap.org/soap/http
Documentation:
```

Figure 5.14: The WSDL for the TCl-Db SOAP service can be found at http://spira.zoology.gla.ac.uk/app/nusoap.

the protocol that builds the interoperability within web services in a platform independent manner, as it is essentially an agreed standard for accessing a web service. The advantage of building web services for interoperability of applications are especially seen in Service Oriented Architectures (SOA). In a SOA the service provider has a service designed for others to use.

Interoperability is a core principle in the development of TCl-Db, since the database was developed for the purposes of interoperability with other databases, TreeBASE specifically, but not exclusively (Tsenov, 2004). To this end, the interfaces described below are available as web services using nuSOAP (Nichol, 2004). The TCl-Db web service provides a WSDL detailing the interface, the operations and the inputs and outputs of the operations. An example of the client code in PHP is given in Table 5.4, to exemplify the use of the service (Figure 5.14). Each of the functions in the WSDL are described briefly below with an example of the expected input and an example output.

Displaying Linked Names and Classifications with Webdot in SOAP

The outputs created by functions `createDot`, `getchildrendot_itis` and `getchildrendot_ncbi` are shown in Figures 5.15 and Figure 5.16.

```
<?php
require_once('./lib/nusoap.php');
// Get inputs
$client = new soapclient('http://localhost/app/nusoap/tclsearchwsdl.php');
$int = array('int'=>'1818'); # AN ITIS or NCBI ID
$param = array('string'=>$_GET['string']);
$name_id = array('name_id'=>$_GET['name_id']);
// Call the functions
$result = $client->call('getName', $param);
$dot = $client->call('createDot', $param);
$itischildrendot = $client->call('getchildrendot_itis', $name_id);
$ncbichildrendot = $client->call('getchildrendot_ncbi', $name_id);
$classification = $client->call('getclassification_itis', $param);
$name = $client->call('getNameByID', $int);
$ids = $client->call('getids', $param);
$assertions = $client->call('getassertions', $param);
$hierarchy = $client->call('gethierarchy', $param);
$synonym = $client->call('getsynonym', $param);
$vernacular = $client->call('getvernacular', $param);
// Display the results
print_r($result);
print_r($dot);
print_r($itischildrendot);
print_r($ncbichildrendot);
print_r($classification);
print_r($name);
print_r($ids);
print_r($assertions);
print_r($hierarchy);
print_r($synonym);
print_r($vernacular);
?>
```

Table 5.4: Example PHP script that calls each of the SOAP functions.

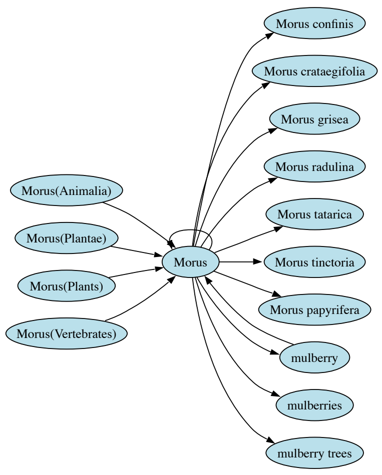


Figure 5.15: WebDot diagram for linked names for the term Morus. From the URL http://spira.zoology.gla.ac.uk/app/nusoap/getWebdotByNameClient.php?name_text=Morus

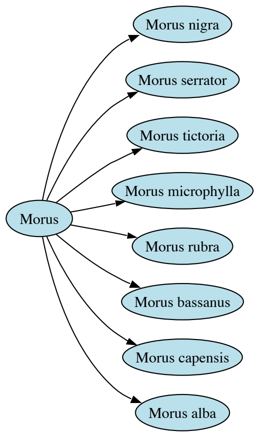


Figure 5.16: WebDot diagram for ITIS children names for the term Morus. From the URL http://spira.zoology.gla.ac.uk/app/nusoap/getchildrenwebdotClient.php?name_id=13107094

SOAP - Basic search

The basic search functions are `getids`, `getName` and `getassertions`.

- `getids` takes a name as input and returns the identifiers at the data source. The XML below is the output from the URL
  http://spira.zoology.gla.ac.uk/app/nusoap/getTCLIDClient.php?string=Pinguinus

```
<response>
   <tcl_name string="Pinguinus" id="13235745" status="valid">
     <SP2K>2393290</SP2K>
     <NCBI>94622</NCBI>
     <Moro>10831</Moro>
     <Amer>10978</Amer>
     <Amer>2854</Amer>
     <pete>10614</pete>
     <Sibl>11334</Sibl>
     <NCBI>94622</NCBI>
     <ITIS>177036</ITIS>
   </tcl_name>
</response>
```

- `getName` does the reverse of `getids` and uses a source database ID to gather the name from TCl-Db.
  http://spira.zoology.gla.ac.uk/app/nusoap/getNameByIDClient.php?int=177036
  The name sources are independent databases and an integer used as an identifier in one database can be used to identify something else in another as shown in the example below.

```
<response>
   <NCBI>tall donkey orchid</NCBI>
   <SP2K>acacia</SP2K>
   <ITIS>great auks</ITIS>
   <ITIS>Pinguinus</ITIS>
   <NCBI>Diuris drummondii</NCBI>
</response>
```

- `getassertions` takes a name as input. Below is the XML output from the URL http://spira.zoology.gla.ac.uk/app/nusoap/tclassertionClient.php?string=Pinguinus

```
<response>
   <tcl_name string="Pinguinus" id="13235745" status="valid">
      <Assertion>
      <nameString>Pinguinus</nameString>
      <dbstring>SP2K</dbstring>
      <IdentifiedBy>2393290</IdentifiedBy>
      <rankString>Genus</rankString>
      <Kingdom>Animalia</Kingdom>
      <parentString>Laridae</parentString>
      </Assertion>
      <Assertion></Assertion>
      <Assertion></Assertion>
      <Assertion></Assertion>
      <Assertion></Assertion>
   </tcl_name>
</response>
```

SOAP - Vernacular/Synonym search

Two functions are provided, `getsynonym` and `getvernacular`. An example output for the vernaculars is given below. This can also be viewed from the URL http://spira.zoology.gla.ac.uk/app/nusoap/tclvernacularClient.php?string=Aves

```
<response>
   <tcl_name string="Aves" id="13232598" status="valid">
      <vernacularString>birds</vernacularString>
      <dbstring>ITIS</dbstring>
      <IdentifiedBy>174371</IdentifiedBy>
      <Kingdom>Animalia</Kingdom>
      <vernacularString>birds</vernacularString>
      <dbstring>NCBI</dbstring>
      <IdentifiedBy>8782</IdentifiedBy>
   </tcl_name>
</response>
```

SOAP - Hierarchical search

The functions `gethierarchy` and `getclassification` provide the hierarchical interface to the database.

- `getclassification_itis` takes a name as input and traverses up the ITIS tree to get the classification to the root. This function uses the materialised paths data for the name and traverses this in a PHP array. The example output below is from the URL http://spira.zoology.gla.ac.uk/app/nusoap/getclassificationClient.php?string=Pinguinus

```
<response>
   <tcl_name string="Pinguinus" id="13235745" status="valid">
     <path>
               Laridae,Ciconiiformes,Aves,Vertebrata,Chordata,Animalia,
     </path>
   </tcl_name>
</response>
```

- `gethierarchy` also takes a name as input. The function uses the nested set data to retrieve the full hierarchy below the search term. This function differs from the the Webdot functions described above, `getchildren_itis` and `getchildren_ncbi` return all the children directly below that node using the parent-child data in the NODE table, whereas the `gethierarchy` returns the direct parent from each data source. The example below is from the URL http://spira.zoology.gla.ac.uk/app/nusoap/tclhierarchyClient.php?string=Pinguinus and has been simplified for clarity.

```
<response>
   <tcl_name string="Pinguinus" id="13235745" status="valid">
     <itis>
       <node id="11648509">
       <child>Pinguinus impennis</child>
       <parent>Pinguinus</parent>
       </node>
       <node id="11648510">
       <child>Pinguinus</child>
       <parent>Laridae</parent>
       </node>
     </itis>
     <ncbi>
       <node id="12153284">
       <child>Pinguinus impennis</child>
       <parent>Pinguinus</parent>
       </node>
       <node id="12153285">
       <child>Pinguinus</child>
       <parent>Laridae</parent>
       </node>
     </ncbi>
     <sp2k>
     </sp2k>
   </tcl_name>
</response>
```

5.5 Summary

This Chapter shows the queries that TCl-Db supports and gives examples of the types of analysis that can be performed on integrated data within TCl-Db. The web tools and applications were developed to search the TCl-Db warehouse of taxonomic names. The tools shown here are examples of the kind of tools that can be developed. The database, however, has a very broad scope and with the ease of development using PHP further applications can be built for the purposes of individual researchers. The examples illustrated here show both a simple standalone web interface and an interface deployed over another database, TreeBASE. The tools are also available as a web service through SOAP, enabling interoperability with other systems. Further work and future considerations will focus on the suggest interface mock up based on Google suggest. Since the version of TreeBASE shown here is out-of-date, a more recent version of the data will be installed.

The following two chapters exemplify further the utility of the database. Chapter 6 shows how the data sources can be compared and reconciled further through the identification of misspellings and homonyms. Chapter 7 highlights the advantages of using TCl-Db to query data in TreeBASE.

Chapter 6

TCl-Db Reconciling data sources

6.1 Summary

Taxonomic data sources, such as the Integrated Taxonomic Information System (ITIS, 2006), the Universal Biological Indexer and Organizer (uBio, 2006) and Species 2000 (Bisby & Smith, 2000) do an exemplary job in providing up-to-date taxonomic data to their respective user communities. As a result, the accessibility of taxonomic data to users has never been easier. Taxonomists continue to invest in their data by focusing on data accessibility (Patterson *et al.*, 2006; Remsen *et al.*, 2006), data management (Polaszek, 2005) and now data quality (Chapman, 2005a,b). TCl-Db is a next step in data availability. It provides a global view of taxonomic names from multiple data sources. The merged data in TCl-Db can be used to determine data quality in terms of accuracy, consistency and completeness within these taxonomic data sources (Fox *et al.*, 1994). Described here are the queries and results of a data cleaning and reconciliation task performed on the class Aves (birds). We have identified spelling inconsistencies, synonym discrepancies, homonyms and classification differences. These data have been used to add links between names in the TCl-Db structure, adding value and providing clarity and consistency to the data provided in TCl-Db.

6.2 Background

As more and more taxonomic data becomes available to the wider user community, focus is beginning to shift towards understanding the distribution and quality of taxonomic data

(Chavan *et al.*, 2005; Embury *et al.*, 2001). Data accuracy, consistency and completeness are issues the taxonomic community are beginning to address (Chapman, 2005a,b). By reconciling taxonomic data, we can begin to understand the quality of the data currently available and deliver more information to our user communities. TCl-Db can be used to identify differences that can handicap non-expert and inexperienced users. Also, reconciling names from several data sources is one of the first steps in a super tree construction, where taxon names used in the trees need to be synonymised (Thomas *et al.*, 2004) to a standard checklist. This chapter shows how TCl-Db can facilitate these tasks.

Integrated Taxonomic Information System (ITIS, 2006), the Universal Biological Indexer and Organizer (uBio, 2006), Species 2000 (Bisby & Smith, 2000) and NCBI are some examples of the successful investment that has been made in the dissemination of taxonomic data on the web. These systems were developed to meet specific user requirements. For example, NCBI provides a taxonomic backbone to the NCBI sequence database GenBank, and the scope of ITIS is limited to taxa of interest to North America. With many more, made to order databases, taxonomic data has never been so readily accessible and taxonomy now has an enormous web presence. The difficulty now is understanding the landscape of taxonomic data, i.e. what data are where? Another difficulty is the accessibility and discovery of heterogeneous data. Data integration and interoperability are now a major focus (Godfray, 2007; Stein & Wieczorek, 2004). There is considerable benefit in combining and merging data from many taxonomic data sources. Aside from providing a single point of entry to taxonomic data, integrated data sources such as TCl-Db enable us to compare data sources side by side to determine and understand data quality and distribution. When combined into a common structure, names from several data sources can be compared to each other to identify differences, inconsistencies and understand data coverage and distribution. Uncovering these data quality metrics (Fox *et al.*, 1994; Wang *et al.*, 1995) gives users the ability to understand, and therefore, use the data better.

In this chapter we exemplify the use of the simplest data cleaning approach, *Verification*. Using the analogy of a spell checker, this type of cleaning approach takes a datum (in this case a taxon name) and evaluates its correctness by comparison to a verified list (in this case the other data sources). Since all names that are identical are reconciled by the integration processes, the process first involves identifying and extracting names unique to individual data sources and then comparing these to each other data source. This kind of data cleaning and reconciliation is exemplified here for the class Aves. This data set was chosen for its manageable size of approximately 10,000 species and also the availability of taxonomic data from many data sources, including digitised checklists from the Early Bird Project (Hackett, 2003). The addition of the checklists offers the opportunity for demonstrating the use of TCl-Db for reconciling multiple name sources, as is often required in supertree analysis.

6.3 Aves Checklist - Data Transformation

A description of the TCl-Db architecture can be found in Chapter 3, and the data transformation processes for the data sources are fully outlined in Chapter 4. Additional data from a number of Aves checklists were made available to us through the Early Bird Project. These data came in the form of flat files and were loaded into individual tables and transformed into the global schema.

Table 6.1 shows the order in which the checklist data were added to the global schema and the number of new Aves names that came in from each source. The table shows that there were over 2000 Aves names that were not in TCl-Db, and the inclusion of the early bird data added not only more assertions, but also more names. Table 6.2 shows the data distribution of each data source by rank. These data were a byproduct from the PL/SQL procedures that were used to add rank data.

Check List	Total Names	New Names Added	Existing Names in TCl-Db
Morony, Bock and Farrand (247)	11,396	659	10,796
Sibley and Monroe(248)	11,909	81	11,850
American Ornithological Union 83 (250)	2741	39	2716
American Ornithological Union 98 (251)	2914	60	2888
Peters (252)	11,218	1221	10,046
NAM980612 (253)	12,018	60	11,974
Bird_Names (256)	9652	101	9560
Clements (259)	96,48	0	9657
Total		2221	

Table 6.1: Content of the Aves Checklists Data. These numbers come from a count on the materialized views used in the transformation of the each sources data into TCl-Db. 2221 new Aves names were added to TCl-Db from these data sources.

6.4 Results

The analyses described below identify unique data (names unique to a single data source), inconsistent data (synonym names where different data sources show different valid names) and

Total	ITIS 14095	NCBI 6386	Sp2000 13985	Peters 11218	NAM 12018	MBF 11396	AOU 98 2741	SibMon 11909	Clements
Superorder		2							
Order	23	36	23	24	22	29			
Suborder	29								
Superfamily		2							
Family	195	169	(153)	(168)	(146)	(166)	(89)		
Subfamily	26	28							
Genus	2169	1430	2264	2128	2081	2048	740		
Species	10103	3990		(8899)	9767	9152	1907	9707	19122
Subspecies	1569	733							
no rank		12	26						

Table 6.2: Summary of the distribution, by rank, of Aves names across the data sources. In brackets are the data where rank information was extrapolated.

missing data (synonyms or vernacular names with no valid name link).

Our investigation started with how much overlap existed between Aves data source. With the inclusion of the checklists, there were eleven distinct data sources for Aves data (ITIS, NCBI, SP200 and the 8 sources shown in Table 6.1). On transformation into the global schema the total number of bird names reconciled within TCl-Db was 26,831. The initial comparison of each data source is given in the Table 6.3. This table displays one aspect of data quality, the relative completeness of each individual data source. The columns represent the percentage overlap in names of that data source in comparison to the other one. We see that 81.7% of Sp2000 names (SP2K) are in NCBI while only 37% of NCBI names are in SP2K. The colour coded columns represent the percent overlap between data sources, red and white shading shows less than 50% overlap and we see that NCBI, AOU83 and AOU98 have the poorest overlap with all other data sources.

In terms of completeness NCBI scores poorly. NCBI contains only 6,386 Aves names from the total 26,831 unique Aves names in TCl-Db. In this respect it is only 23.8% complete. Although this number initially seems very low, it should be noted that NCBI data represents species for which nucleotide or amino acid sequence information is available. Therefore, this number actually reflects the fact that 23.8% of Aves species have sequence data. Given this context, the data can actually be considered 100% complete, as all known sequences for Aves are most likely included in GenBank. Since, data quality in terms of completeness can not be measured independent of the data sources' data scope, and we focus instead, on data quality

	ITIS	NCBI	SP2K	MBF	SM	AOU98	AOU83	Peters	Clements
ITIS		37	99.2	77.7	83.5	18.9	19.7	69.1	66.8
NCBI	81.7		81.3	75	77.6	28.2	29.2	70.3	55.4
SP2K	100	37.1		75	84	19	19.7	69.4	67.3
MBF	91.9	41.8	91.5		90.8	23.8	23.7	89.3	72.4
SM	98.6	41.5	98.5	87.2		22	22.2	80.4	78.4
AOU98	97	65.5	96.6	99.1	95.5		94.6	87.4	65.8
AOU83	56.9	38.6	55.8	56.3	53.7	52.9		50.2	76.8
Peters	86.5	39.8	86.1	90.8	85.2	21.3	21.4		66.9
Clements	48.8	18.3	48.7	42.9	48.5	9.3	19.6	39	

Table 6.3: The percentage overlap of taxon names in each pair of data sources. For example, 37% of names in NCBI are also in ITIS, whereas 81.7% of names in ITIS are also in NCBI. This all against all comparison for Aves data sources includes the checklists from the early bird project: MBF is (J.J. Morony *et al.*, 1975), SM is (Monroe & Sibley, 1997), AOU 98 and AOU 83 are (American Ornithological Union, 1998) and American Ornithological Union, 1983), Peters is (Peters, 1987), and Clements is (Clements, 2000). The data sets with more than 75% overlap are coloured yellow, data sets with between 50% and 75% overlap are coloured green, 25% to 49% are coloured red and less than 25% are coloured white. The SQL was a simple boolean query on two subsets of the assertion data. The SQL query is given as Query B1 in Appendix B.1.

in terms of accuracy and consistency. The remainder of this analysis examines the NCBI unique names in detail. Since sequence data is playing a more significant role in defining and identifying species (Hebert *et al.*, 2004; Mallet & Willmott, 2003), an understanding of the quality of taxonomic data within this increasingly important data source, and how it compares to more traditional data sources, is appropriate at this time. The data warehouse approach used in TCl-Db enables these kinds of analyses to be performed efficiently.

Aves in NCBI

An initial comparison of NCBI and ITIS returned 1169 unique NCBI names. Our aim here was to determine how many of these names could be resolved further and linked to names in other data sources. Some names unique to NCBI were easily accounted for using simple SQL queries. NCBI contains sequence data for extinct species, some of which are not included in ITIS. These species are listed in Table 6.4. Differences in classification also account for some of the unique names. For example in NCBI there are 20 names of the rank sub-family that are not in ITIS. 39 are names that ITIS treated as synonyms, which NCBI considered to be valid. A selection of these are listed in Table 6.5.

Valid name	Vernacular	NCBI Tax ID	Class
Aegotheles novaezealandiae		191447	Aves
Anomalopteryx didiformis	little bush moa	8811	Aves
Aptornis defossor	South Island adzebill	54366	Aves
Dinornis novaezealandiae	large bush moa	8818	Aves
Dinornis robustus		314500	Aves
Dinornis struthoides	slender bush moa	237965	Aves
Euryapteryx curtus	costal moa	230980	Aves
Euryapteryx geranoides	stout-legged Moa	314499	Aves
Fulica chathamensis	New Zealand coot	54568	Aves
Harpagornis moorei	New Zealand giant eagle	307641	Aves
Megalapteryx benhami		328612	Aves
Megalapteryx didinus	South Island Tokoweka	8813	Aves
Pachyornis elephantopus	heavy-footed moa	8815	Aves
Pachyornis australis	crested moa	239969	Aves
Pachyornis mappini	Mappins moa	239970	Aves
Thambetochen chauliodous	moa-nalo	107030	Aves

Table 6.4: NCBI extinct species not in ITIS. These data were downloaded from Entrez at http://www.ncbi.nlm.nih.gov/Taxonomy/taxonomyhome.html/index.cgi?chapter=extinct

NAME_ID	ITIS Synonym/NCBI Valid Names	NAME_ID	ITIS Valid name
13370347	*Cyanopica cyanus*	13290971	*Cyanopica cyana*
13421691	*Syrmaticus reevesi*	13286348	*Syrmaticus reevesii*
13389945	*Catreus wallichi*	13235716	*Catreus wallichii*
13368910	*Anser canagica*	13231876	*Anser canagicus*
13502780	*Ptilinopus melanospil*	13236835	*Ptilinopus melanospila*
13383217	Troglodytinae	13235043	Troglodytidae
13385669	Batrachostomatidae	13284858	Batrachostomidae
13482607	Mesitornithidae	13289249	Mestiornithidae
13444945	*Thalassarche melanophris melanophris*	13287984	*Thalassarche melanophris*
13386024	*Columba inornata wetmorei*	13235949	*Columba inornata*
13500532	*Poecile carolinensis extimus*	13287820	*Poecile carolinensis*
13426291	*Tetrao tetrix tetrix*	13286352	*Tetrao tetrix*
13457566	*Anas flavirostris flavirostris*	13235934	*Columba flavirostris flavirostris*
13432409	*Cyanopica cyanus gili*	13290971	*Cyanopica cyana*

Table 6.5: A few of the NCBI names that are not considered valid names in ITIS but are represented as synonyms. The SQL that identified these synonyms was query B2 in Appendix B.1.

6.4.1 Classification Differences

When the NCBI unique names were quantified by rank, we found that some of these unique names fell into ranks not included in ITIS, as stated above for the rank subfamily. The two superorder names used in NCBI are: Palaeognathia (Palaeognathae) Huxley, 1867 (Pygraft, 1900) and Neognathia (Neognathae) Huxley, 1867 (Pygraft, 1900). The ITIS classification for the class Aves goes directly to order level. However, these two names follow the accepted hypotheses that modern birds (subclass Neornithes) subdivide into these named superorders (Edwards *et al.*, 2005), and ITIS simply does not include the rank superorder. Peters, Morony, Bock and Farrand (MBF), ITIS and Sp2000 go from the class Aces directly to Order, while Sibley and Monroe (SM), and the AOU data sources do not contain Order data (see Table 6.2).

Of the 36 orders in NCBI, fourteen are unique to NCBI and twelve of these are considered to be synonyms in other data sets: Caprimulgiformes (Strigiformes), Rheiformes, Casuariiformes, Apterygiformes (Struthioniformes) and Sphenisciformes, Gaviiformes, Podicipediformes, Procellariiformes, Pelecaniformes, Falconiformes, Charadriiformes, Phoenicopteriformes (Ciconiiformes) (Sibley & Ahlquist, 1990). The two remaining orders are Dinornithiformes which includes two families, six genera and ten species which are all extinct moas and unique to NCBI. Opisthocomiformes, which includes the family Opisthocomidae, contains one genus *Opisthocomus* Illiger, 1811 and one species *Opisthocomus hoazin* Muller, 1776. These names exist in ITIS under the family Cuculiformes.

The two superfamily names unique to NCBI are Passeroidea and Corvoidea. In NCBI, the Passeroidea contain the following families: Alaudidae, Paramythiidae, Nectariniidae, Passeridae, Fringillidae and Melanocharitidae; while the Corvoidea contains the families Orthonychidae, Vireonidae, Laniidae, Corvidae, Callaeatidae and Irenidae. These names exist in ITIS under the order Passeriformes, and again ITIS does not include the rank superfamily.

The family names Aptornithidae, Emeidae, Aepyornithidae and Dinornithidae represent classification of extinct species. Seven of the eighteen family names were found to be synonyms in ITIS. These are: Dromaiidae (Casuariidae), Diomedeidae, Pelecanoididae (Procellariidae), Cathartidae (Ciconiidae), Haematopodidae (Charadriidae), Stercorariidae (Laridae) and Alcidae (Laridae). The NCBI family Batrachostomatidae contains one genus and one species *Batrachostomus cornutus*. This name is found in ITIS under the classification Batrachostomus/Batrachostominae/Podargidae. The NCBI family Pteroclidae contains two genera and six species, these are each in ITIS but the family name is spelt Pteroclididae.

Only ITIS and NCBI have subfamilies for Aves. ITIS has 26 and NCBI has 28, but only 8 subfamilies are common to both databases. Table 6.6 gives these names, and shows that both NCBI and ITIS disagree above family level.

Subfamily	ITIS family	NCBI family	parent name ITIS family	parent name NCBI family
Pandioninae	Accipitridae	Accipitridae	Ciconiiformes	Falconiformes
Carduelinae	Fringillidae	Fringillidae	Passeriformes	Passeroidea
Estrildinae	Estrildidae	Estrildidae	Oscines	Passeriformes
Viduinae	Estrildidae	Estrildidae	Oscines	Passeriformes
Fringillinae	Fringillidae	Fringillidae	Passeriformes	Passeroidea
Drepanidinae	Fringillidae	Fringillidae	Passeriformes	Passeroidea
Accipitrinae	Accipitridae	Accipitridae	Ciconiiformes	Falconiformes
Phasianinae	Phasianidae	Phasianidae	Galliformes	Galliformes

Table 6.6: Subfamily names common to both NCBI and ITIS. Although the family names are in agreement, the classification above family does not agree.

Next, we looked at how many genera common to NCBI and ITIS were classified into different families (Table 6.7). The query used both the NCBI and ITIS classifications and is shown Appendix B.1, query B3.

This query returns 534 genera that have a different parent name within the ITIS classification. Of these, 327 are subfamily names in NCBI with all but six of these having the same family in ITIS. In the remainder, 181 are family names and twenty-six are of unknown rank. We checked how many of the 181 family names were synonyms using the query given in B4, Appendix (B.1), returning the data in Table 6.7. The genus *Sapayoa* (Tyrannidae in NCBI) is the only Incerta_sedis (uncertain classification), leaving 148 genera classified differently in NCBI and ITIS. This query also returned homonyms, i.e., identical names that apply to different taxa. *Bartramia, Batis, Oenanthe, Prunella, Morus* and *Arenaria* are avian genera that are also valid genera in the plant kingdom. Homonyms can cause considerable confusion when performing hierarchical queries as a query by name in these cases returns both plant and bird species. Using a simple query, we can identify all these duplicated names in each hierarchy. These queries were extended to include data in the source schemas, which discriminates between homonyms and database duplications. The queries used to gather these homonyms were replicated into a materialized view (stored query) for both ITIS and NCBI.

Storing multiple classifications and performing hierarchical queries is also useful when differences need to be validated, i.e., where NCBI and ITIS disagree on synonymy; for example, the family names Casuariidae (cassowaries) and Dromaiidae (emus) that have been linked together by synonymy. These are both valid names according to NCBI, however, most other data sources

Genus Name	NCBI Family	ITIS Family
Aethia	Alcidae	Laridae
Alca	Alcidae	Laridae
Alle	Alcidae	Laridae
Bonasa	Tetraonidae	Phasianidae
Brachyramphus	Alcidae	Laridae
Catharacta	Stercorariidae	Laridae
Cathartes	Cathartidae	Ciconiidae
Centrocercus	Tetraonidae	Phasianidae
Cepphus	Alcidae	Laridae
Cerorhinca	Alcidae	Laridae
Coragyps	Cathartidae	Ciconiidae
Dendragapus	Tetraonidae	Phasianidae
Diomedea	Diomedeidae	Procellariidae
Dromaius	Dromaiidae	Casuariidae
Falcipennis	Tetraonidae	Phasianidae
Fratercula	Alcidae	Laridae
Gymnogyps	Cathartidae	Ciconiidae
Haematopus	Haematopodidae	Charadriidae
Lagopus	Tetraonidae	Phasianidae
Pelecanoides	Pelecanoididae	Procellariidae
Phoebetria	Diomedeidae	Procellariidae
Ptychoramphus	Alcidae	Laridae
Stercorarius	Stercorariidae	Laridae
Synthliboramphus	Alcidae	Laridae
Tetrao	Tetraonidae	Phasianidae
Tetraogallus	Tetraonidae	hasianidae
Tympanuchus	Tetraonidae	Phasianidae
Uria	Alcidae	Laridae
Vultur	Cathartidae	Ciconiidae
Agriocharis	Phasianidae	Meleagrididae
Batrachostomus	Batrachostomatidae	Batrachostomidae
Mesitornis	Mesitornithidae	Mestiornithidae

Table 6.7: Listed above are the thirty-two genera out of 181 that are common to ITIS and NCBI but classified differently. In the top section the NCBI family names are synonyms. The three ITIS family names in the section below are synonyms.

show Casuariidae as the current accepted name, and link Dromaiidae to it as a synonym. This link stems from the reclassification of the emus which were formerly classified in their own family, Dromaiidae and later added to Casuariidae. This was determined by examining the children, as shown in Figure 6.1. The first graph shows the ITIS children for Casuariidae and the second shows that the children in NCBI do not include the genus *Dromaius*. The Sibley and Monroe classification agrees with the ITIS classification and can be used to validate the link created between two valid names within TCl-Db.

6.4.2 Spelling

Next, we examined the accuracy of the names in NCBI. The examples above highlighted not only classification differences between NCBI and ITIS, but also spelling discrepancies. Specifically, we were interested in determining the number of names that were not reconciled at the outset, due to differences in spelling. Using the Agrep algorithm (Wu & Manber, 1992), we compared the unique names in NCBI against ITIS names. Agrep is a string searching program that performs approximate pattern matching. Agrep implements several different algorithms for string matching, including a variant of the Boyer-Moore algorithm and the bitap algorithm based on the shift-or algorithm of Baeza-Yates and Gonnet (Navarro, 2001; Wu & Manber, 1992). Agrep takes as input an approximate string (or pattern) and uses the inbuilt string matching algorithms to find that string in a given text file. Using Agrep, names unique to NCBI were compared against ITIS names, allowing for mismatches. Agrep originally found 202 potential matches and this list was manually inspected to give the data in Table 6.8. Of these Agrep matches, 101 (˜1.6% of the 6386 NCBI Aves) names were found to be potentially misspelt.

These names and the ITIS matches are shown in Table 6.8, with the spelling differences highlighted. Twenty-two are genus names (green in Table 6.8), three are family names (blue in Table 6.8) and the remaining are species names. The refinement process was largely manual and removed approximate matches found between a subfamily ending in -idae and a family ending in -inae. These could be easily identified automatically with simple rules in a PL/SQL script. For example, a rule can be used to rule out matches where the matching string is the parent name of the search string.

Two matches in the genus epithet were found, *Pipile Nattereri* matched to the ITIS name *Pipra nattereri* and *Turdus abyssinicus* matched the ITIS name *Turtur abyssinicus*. The visual check could not tell if these were misspellings or actually different genera with the same specific

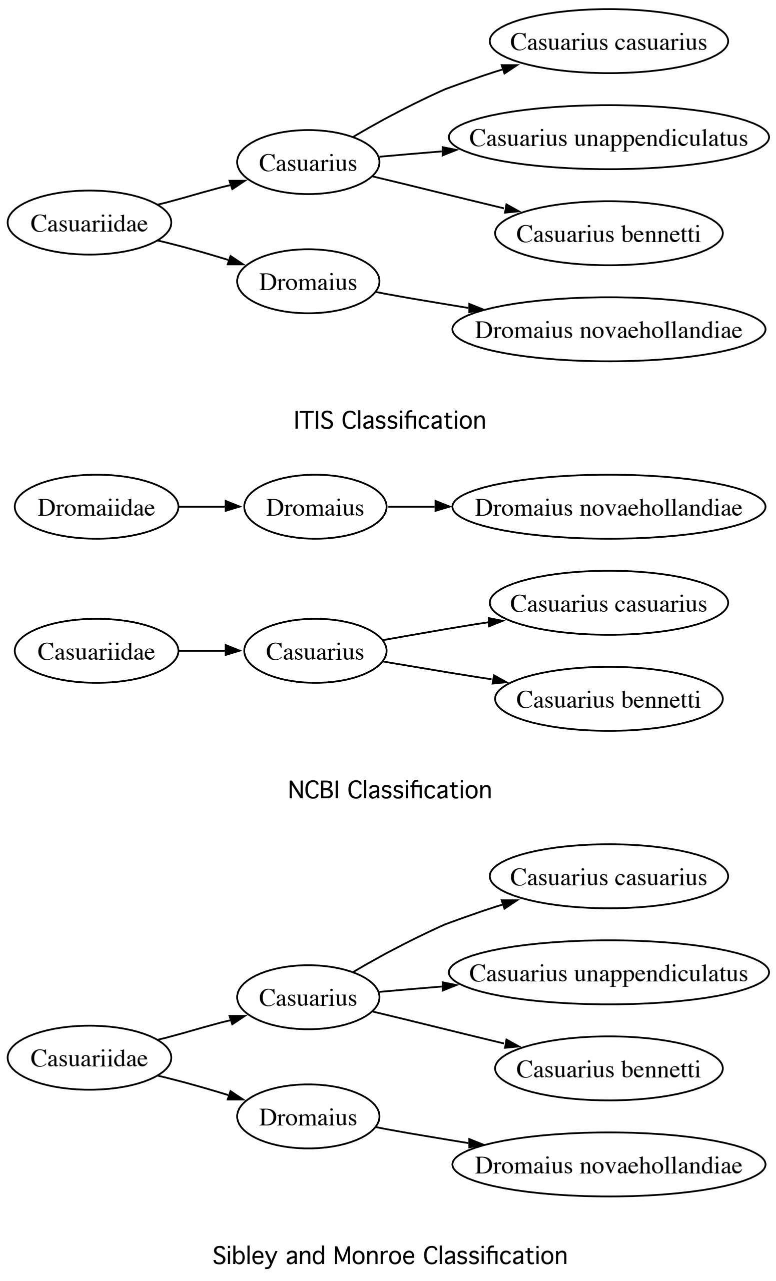


Figure 6.1: Multiple Classifications of Casuariidae.

epithet, so these were reconciled using distribution data, i.e., since NCBI had more than one name in those genera, it was unlikely that the Agrep matches represented misspellings. This analysis found many false positives which could only be identified and validated by manual inspection, full automation of this process would not be feasible.

Most of the names in Table 6.8 are species names. Subspecies names were not included in the analysis as the Agrep algorithm is limited to strings of twenty-seven characters or less when searching with a mismatch. To try and get round this, a script was used to first chop the string to the twenty-seven character limit then add the number of characters removed to the mismatch, up to a maximum of eight. For example, *Malurus leucopterus leuconotus* would be chopped to the string "Malurus leucopterus leucono" allowing for a mismatch of six. This method did not match any subspecies names to any other subspecies and most matches were made to the parent species name. A total of 622 subspecies were not included in the Agrep test. Since Agrep could not be used for all names in this data set, the Soundex algorithm (Zobal & Dart, 1996) was then tested. Soundex differs from Agrep in that it does not string match but converts each string into a code where phonetically similar strings get the same codes. Soundex did not perform particularly well compared to Agrep. Taxonomic names are Latin and since Soundex codes each name by English pronunciation, this was not unexpected. The algorithm did usually find matches, e.g., *Bradypterus baboecola* matched *Bradypterus baboecala*, but also twenty-one other names making the data too noisy to parse automatically. A combination of string matching for genus and phonetic matching for specific epithet was slightly less noisy, however, this combination did not perform any better than string matching alone and did not provide any additional data.

	NCBI Spelling	ITIS Spelling
1	*Illadopsis pyrrhopter**um***	*Illadopsis pyrrhopter**a***
2	*No**r**thura maculosa*	*Nothura maculosa*
3	*Criniger ochraceus*	*Criniger o**liv**aceus*
4	*Doryfera ludovic**i**ae*	*Doryfera ludovicae*
5	*Artamus leucor**h**ynchus*	*Artamus leucorynchus*
6	*Seicercus xanthoschist**us***	*Seicercus xanthoschist**o**s*
7	*Carduelis yarellii*	*Carduelis ya**r**rellii*
8	*Anser canagica*	*Anser canagicus*
9	*Thamnolea cinnamomeiventris*	*Thamnol**a**eacinnamomeiventris*
10	*Certhilauda erythroclamys*	*Certhilauda erythroc**h**lamys*
11	*Thinocorus orbignyanus*	*Thinocorus orbigny**i**anus*
12	*Taenopygia guttata*	*Taen**i**opygia guttata*
13	*Myioborus brunn**e**iceps*	*Myioborus brunniceps*
14	Dendrocolaptidae	Dendrocolapt**er**idae
15	*Emberiza imp**e**ltuani*	*Emberiza impetuani*
16	*Icterus gracean**e**ae*	*Icterus gracea**n**nae*
17	*Cisticola fulvicapilla*	*Cisticola fulvicapillus*
18	*Rhabdornis mysticalis*	*Rhabdornis mystacalis*

19	*Francolinus levaillantoides*	*Francolinus levail**l**iantoides*
20	*Calor**h**amphus fuliginosus*	*Calor amphus fuliginosus*
21	*Chlamydera lauterbachi**i***	*Chlamydera lauterbachi*
22	*Schistochlamys melanop**s**is*	*Schistochlamys melanopis*
23	Platysterira	Platysteira
24	*Ptilogonys cinereus*	*Ptil**i**ogonys cinereus*
25	*Loboparadis**a**ea sericea*	*Loboparadisea sericea*
26	*Upucerthia dumeteria*	*Upucerthia dumetaria*
27	*Ketupa ketupa*	*Ketupa ketupu*
28	*Pterglossus azara*	*Pter**o**glossus azara*
29	Tachybap**th**us	Tachybaptus
30	*Tricholaema lac**h**rymosa*	*Tricholaema lacrymosa*
31	*Ep**h**thianura tricolor*	*Epthianura tricolor*
32	*Amytornis striatus*	*Amytornis barbatus*
33	*Rhipidura hyperthra*	*Rhipidura hyper**y**thra*
34	*Aerodramus terraereginae*	*Aerodramus terraereginus*
35	Cactospiza	Charitospiza
36	*Serinus canicolis*	*Serinus canico**l**lis*
37	*Dives warsz**w**ewiczi*	*Dives warszewiczi*
38	*Northellia haematogaster*	*Nort**hi**ella haematogaster*
39	*Chamaeza mollisima*	*Chamaeza moll**iss**ima*
40	Calorhamphus	Colorhamphus
41	*Parus ater*	*Parus afer*
42	*Pitta guajara*	*Pitta guajana*
43	Calicalius	Calicali**c**us
44	Jabouillea	Jabouill**e**ia
45	Mesitornithidae	Mes**ti**ornithidae
46	*Certhilauda brevirostris*	*Certhilauda curvirostris*
47	*Pterocnemia pennata*	*Pter**oi**cnemia pennata*
48	Loboparadis**a**ea	Loboparadisea
49	*Liosceles thorasicus*	*Liosceles thoracicus*
50	*Basileuterus rubifrons*	*Basileuterus rufifrons*
51	*Poospiza hispaneolensis*	*Poospiza hispaniolensis*
52	Corv**o**idea	Corvidae
53	*Volatin**a** jacarina*	*Volatin**ia** jacarina*
54	*Lophura erythropthalma*	*Lophura erythrop**h**thalma*
55	*Pteruthius xanthochlo**ris***	*Pteruthius xanthochlo**rus***
56	*Puffinus nativitat**us***	*Puffinus nativitatis*
57	*Aerodramus salangan**a***	*Aerodramus salanganus*
58	*Taenopygia bichenovii*	*Taen**i**opygia bichenovii*
59	*Speleaornis chocolatinus*	*Spelaeornis chocolatinus*
60	*Cyanopica cyanus*	*Cyanopica cyana*
61	*Cisticola cherina*	*Cisticola cherinus*
62	*Jabouillea danjoui*	*Jabouill**ei**a danjoui*
63	*Turdus falklandii*	*Turdus fal**c**klandii*
64	*Pterodroma deserta*	*Pterodroma incerta*
65	*Cercotrichas quadrivi**r**igata*	*Cercotrichas quadrivirgata*
66	Pterocnemia	Pter**oi**cnemia
67	*Calicalius madagascariensis*	*Calicali**c**us madagascariensis*
68	Ep**h**thianura	Epthianura
69	*Pachycephala hyperthra*	*Pachycephala hyperythra*
70	*Pelecanoides magellani**cus***	*Pelecanoides magellani*
71	*Buarremon brunneinucha*	*Buarremon brunneinuchus*
72	*Mionectes macconnelli**i***	*Mionectes macconnelli*
73	Gallirex	Gallicrex
74	Raphidura	R**h**aphidura
75	Basileuterus tristiatus	Basileuterus trist**r**iatus
76	Taenopygia	Taen**i**opygia
77	Northura	Nothura
78	Cecropis	Crecopsis

79	Volatina	Volatinia
80	*Francolinus africanus*	*Francolinus africans*
81	*Basileuterus crysogaster*	*Basileuterus chrysogaster*
82	*Neochen jubatus*	*Neochen jubata*
83	*Platysterira cyanea*	*Platysteira cyanea*
84	*Chrysothlypis chrysomelas*	*Chrysothlypis chrysomelaena*
85	*Caprimulgus seriocaudatus*	*Caprimulgus sericocaudatus*
86	Lophotis	Lophornis
87	*Saurothera vielloti*	*Saurothera vieilloti*
88	Speleaornis	Spelaeornis
89	*Picoides dorsalis*	*Picoides borealis*
90	*Sephanoides sephanoides*	*Sephanoides sephaniodes*
91	Philetarius	Philetairus
92	*Tachybapthus ruficollis*	*Tachybaptus ruficollis*
93	Thamnolea	Thamnolaea
94	*Acrocephalus sirpaceus*	*Acrocephalus scirpaceus*
95	*Saxicola rubertra*	*Saxicola rubetra*
96	*Raphidura leucopygialis*	*Rhaphidura leucopygialis*
97	*Rallus philippiensis*	*Rallus philippensis*
98	Acanthagenys	Acanthogenys
99	*Philetarius socius*	*Philetairus socius*
100	Pterglossus	Pteroglossus
101	*Acanthagenys rufogularis*	*Acanthogenys rufogularis*

Table 6.8 Agrep matches in ITIS for unique NCBI names.
Locations of differences are underlined and highlighted in bold.
The genus and family names are coloured green and blue, respectively.

The remaining generic names, after removing the twenty-two spelling discrepancies and eight extinct genera, are listed in Table 6.9. The remaining species and subspecies names that were not found to be misspellings, extinct or located within these unique genera, are likely to be genuinely unique to NCBI. Twenty-four names were of the structure "Genus sp." i.e., *Grus sp.*. These names are valid in NCBI and stand for species not yet taxonomically published with a specific epithet and representing an increasing number of unidentified sequences (Nilsson *et al.*, 2005). When looking more closely at the subspecies, it was found that for 312 of the 622 subspecies, the parent species names existed in ITIS. Similarly, for 149 of the 407 unique species names, the parent genus name existed in ITIS. These data represent the distributional biases in the two databases. Further analysis of these names was beyond the scope of the data within TCl-Db. However, for the remaining unique NCBI names, sequence accession numbers, and Digital Object identifiers (DOI) for articles publishing those sequences were extracted from the NCBI sequence records and added to TCl-Db, they are presented to users in the interface in order to ease the manual inspection of each, see section 6.5 and Figure 6.2.

Genus	Species name
Guaruba	*Guaruba guarouba*
Xanthopsar	*Xanthopsar flavus*
Acanthis	*Acanthis flammea*
Halocyptena	*Halocyptena microsoma*
Eulipoa	emphEulipoa wallacei
Phonygammus	*Phonygammus keraudrenii*
Schistolais	*Schistolais leontica*
	Schistolais leucopogon
Ruwenzorornis	*Ruwenzorornis johnstoni*
Turdampelis	*Turdampelis subalaris*
	Turdampelis cryptolophus
Pygochelidon	*Pygochelidon cyanoleuca*
Pseudhirundo	*Pseudhirundo griseopyga*
Afrotis	*Afrotis afra*
	Afrotis afraoides
Diopsittaca	emphDiopsittaca nobilis
Ptaiochen	*Ptaiochen pau*
Creadion	*Creadion carunculatus*
Cossyphicula	*Cossyphicula roberti*
Criniferoides	*Criniferoides leucogaster*
Chalcites	*Chalcites lucidus*
Diphyllodes	*Diphyllodes magnificus*
	Diphyllodes respublica
Chalcites	*Chalcites minutillus*
	Chalcites basalis
Aidemosyne	*Aidemosyne modesta*
Northellia	*Northellia haematogaster*
Rhynochetus	*Rhynochetus jubata*
Orthopsittaca	*Orthopsittaca manilata*
Terenotriccus	*Terenotriccus erythrurus*
Emeus	*Emeus crassus*
Primolius	*Primolius maracana*
Houbaropsis	*Houbaropsis bengalensis*
	Primolius couloni
	Primolius auricollis
Stizorhina	*Stizorhina finschi*
Hoplopterus	*Hoplopterus spinosus*
Stictocarbo	*Stictocarbo punctatus*
Platyspiza	*Platyspiza crassirostris*
Cyclorrhynchus	*Cyclorrhynchus psittacula*
Lunda	*Lunda cirrhata*
Asarcornis	*Asarcornis scutulata*
Speculanas	*Speculanas specularis*
Ptyonoprogne	*Ptyonoprogne fuligula*
	Stizorhina fraseri
Leistes	*Leistes militaris*
Mullerornis	*Mullerornis agilis*
Lissotis	*Lissotis melanogaster*
	Lissotis hartlaubii
Nesoenas	*Nesoenas mayeri*
Phaeothlypis	*Phaeothlypis fulvicauda*
Parisoma	*Parisoma subcaeruleum*
Schistocichla	*Schistocichla leucostigma*

Table 6.9: 43 genus names unique to NCBI, after accounting for extinct genera and misspellings. The species which they contain are also listed here.

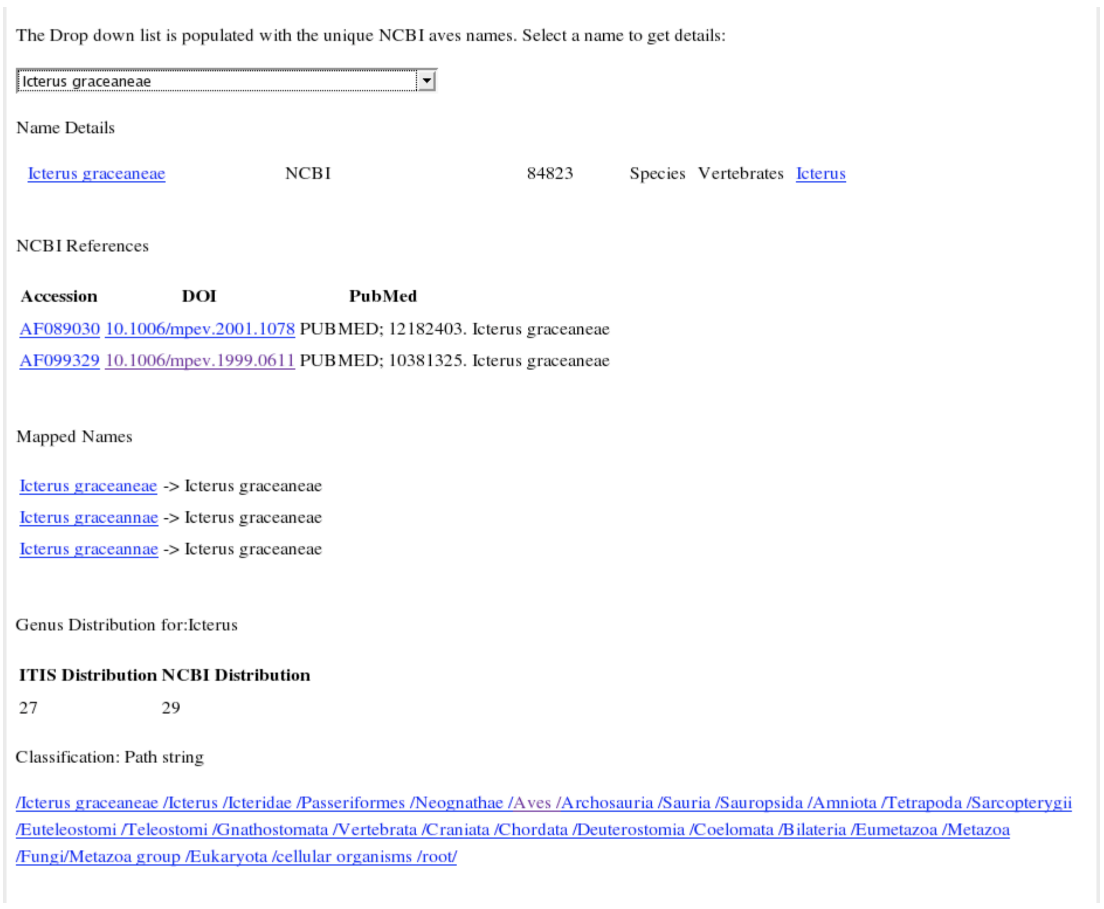
6.5 Data Cleaning and Presentation

Data cleaning is an important aspect of data integration. The quality of data within the data sources reflects the quality of data in TCl-Db. While some data is cleaned on transformation, the data analysis described above shows how such queries can be used for further integration i.e., explicating links that were previously not obvious, such as the link between Opisthocomiformes and Cuculiformes, for example. This data cleaning adds value and validates the links that are created within TCl-Db.

We chose not to correct the misspellings given in Table 6.8, since this would assume that all ITIS spellings are correct. Instead, the two names are linked together in the same way that synonyms are linked to valid names. This way, a search on one spelling will return the alternative spelling. The classification differences between NCBI and ITIS reflect the different schools of thought which present valid hypotheses that are not necessarily incorrect. Therefore, removing the name Dromaiidae from the NCBI classification and moving its children to reflect the other classifications would be inappropriate. However, linking the data together creates transparency by potentially dispelling any confusion that could arise.

One issue that has not been addressed is how the data and queries that have been presented here are performed on other data sets, updated, maintained and delivered to user communities. This analysis could be done in TC-Db using any generic name source. A set of names from phylogenetic trees, for example, can be synonymised using simple SQL queries. The data presented were derived using SQL queries, highlighted by the few examples included in Appendix B.1. SQL is relatively easy to learn, however, we acknowledge that it is difficult to master and efficient queries require an intimate understanding of the database schema. Building simple efficient queries is easy for developers, but considerable development effort would be required to make this kind of analysis simpler and accessible to others. The examples given here present the ability of TCl-Db, given its structure and data content, to perform large scale data quality analyses. The TCl-Db database is available for direct SQL access via iSQL at `http://spira.zoology.gla.ac.uk:5561/isqlplus/`. The Aves example presented here shows that these analyses are possible within a data warehouse like TCl-Db, while these queries could not be performed using the interfaces provided by the individual data sources or through systems like uBio and Sp2000.

A simple search interface has been provided to allow users to search through the data presented in TCl-Db at `http://spira.zoology.gla.ac.uk/search_tcl.php`, which is described



The Drop down list is populated with the unique NCBI aves names. Select a name to get details:

Icterus graceaneae

Name Details

Icterus graceaneae	NCBI	84823	Species	Vertebrates	Icterus

NCBI References

Accession	DOI	PubMed
AF089030	10.1006/mpev.2001.1078	PUBMED; 12182403. Icterus graceaneae
AF099329	10.1006/mpev.1999.0611	PUBMED; 10381325. Icterus graceaneae

Mapped Names

Icterus graceaneae -> Icterus graceaneae
Icterus graceannae -> Icterus graceaneae
Icterus graceannae -> Icterus graceaneae

Genus Distribution for:Icterus

ITIS Distribution	NCBI Distribution
27	29

Classification: Path string

/Icterus graceaneae /Icterus /Icteridae /Passeriformes /Neognathae /Aves /Archosauria /Sauria /Sauropsida /Amniota /Tetrapoda /Sarcopterygii /Euteleostomi /Teleostomi /Gnathostomata /Vertebrata /Craniata /Chordata /Deuterostomia /Coelomata /Bilateria /Eumetazoa /Metazoa /Fungi/Metazoa group /Eukaryota /cellular organisms /root/

Figure 6.2: The interface presenting the data collected for NCBI Unique names http://spira.zoology.gla.ac.uk/ncbi_aves_ref.php

in detail in the previous chapter. The interface is designed for users who wish to view combined taxonomic data, and allows them to perform relatively loose searches and follow links to take them to the information they require. Experts using specific search terms may also find the combined view of the data useful as an initial search before performing searches in other databases. Some of the cleaning and validation data described above is also presented at `http://spira.zoology.gla.ac.uk/aves.html`. From this page there are links to several forms presenting the data from specific queries. For example, a form has been built for the NCBI unique names. These names are presented in a pull down menu and details that have been gathered are returned to the user (see Figure 6.2). Similarly, for the genera in NCBI and ITIS that are classified in different families, a simple comparison interface has been developed to allow users to view the classifications side by side.

6.6 Conclusions

We now understand more clearly the main differences between NCBI and ITIS data and we are better equipped to find these differences. With this knowledge, we can use the data better. For example, knowing that only approximately 18% of known Aves species are represented in GenBank we can better judge species assignments that are based on sequence searches (Hebert *et al.*, 2004). Understanding the distributional biases within databases has applications for users in ecology and conservation, where the use of names from only one database may be inappropriate.

TCl-Db contains integrated, reconciled taxonomic data from multiple data sources. At a basic level, a combined, global view of taxonomic data is presented to users. A combined view of data in a single database enables data validation in terms of corroborating the spelling, status or classification of any given taxonomic name. This is one of the main advantages of the data warehouse approach. The queries performed and described here for the class Aves have identified data that do not reconcile and inconsistencies that can cause confusion. The value added data from these queries enhances further the data content in TCl-Db, creating links across spelling differences and highlighting synonym and classification differences, and thus improving clarity of the data delivered in TCl-Db. Such data analyses are only possible when all data sources are available in a single structure and the data can be compared side by side. This chapter highlights an analysis that is an important initial step in our understanding of data quality and distribution. The following chapter goes on to show the importance of taxonomic data quality and coverage in a phylogenetic database and the effect on data retrieval.

Chapter 7

Using TCl-Db to Improve the Querying of TreeBASE

7.1 Summary

At the outset of TreeBASE (Morell, 1996) design a decision was taken to shelve the issue of taxonomy and as a result, it is fair to say that TreeBASE under performs taxonomically. The database is not taxonomically intelligent and queries do not translate to return all relevant hits. A biologist expects a query on a higher taxa name to translate hierarchically, i.e. return all data contained within the original search term. Likewise, a vernacular query should translate to the accepted name and both queries should be performed automatically for the user. Here, we analyse the queries performed on TreeBASE thus far. We show that vernacular and hierarchical queries are common searches performed by users. The poor performance of these queries displays the importance of biological taxonomy for information retrieval. We use the TCl-Db database to exemplify how the inclusion of taxonomy overcomes the poor data retrieval users are currently experiencing.

7.2 Introduction

In previous chapters we have shown that some classifications do not support some commonly used ranks and that data coverage varies across the taxonomic data sources. While it would be unfitting to apply one classification to TreeBASE, without a classification, TreeBASE does not effectively support higher taxon queries. However, with a taxonomy, it is possible to perform a search using terms linked by association and content. There are many taxonomic databases, electronically available, that can easily be included into a phylogenetic data store. The reasons for TreeBASE not including a taxonomy are now outdated and a simple solution is presented in the form of TCl-Db.

7.3 Background

Currently, systematists prefer to gather the data they require for their analysis through literature searches. In most cases, once data are retrieved, the search results are examined by eye to determine if they contain the phylogenetic data of interest. Unlike the major sequence databases, phylogenetic tree data does not have to be deposited in a database before it can be published. Currently, the deposition of data in TreeBASE has been voluntary. Also, TreeBASE is not used because data are difficult to retrieve using search terms that are intuitive to users. Although TreeBASE provides a Taxon name search, the returned data are often incomplete. The example given in Section 1.5 for the query term “Aves”, shows that data can only be retrieved by exact or partial text matching on taxon names.

Our hypothesis that an integrated taxonomic data source could alleviate the problems of using taxonomic names to retrieve data from TreeBASE is tested through a comparison of the data retrieval of a set of taxon queries performed on a local copy of TreeBASE, and the same queries performed through TCl-Db tables linked to TreeBASE.

Examination of the taxon query logs shows that the taxonomic capacity of TreeBASE is ineffective. The types of queries performed using TreeBASE and the results returned are analysed. In the first section of this chapter we examine the taxon queries that have been performed on the TreeBASE user interface and inspect the retrieval capacity of these queries. These data are then compared to the results found by searches mediated by TCl-Db. Queries performed through TCl-Db show marked improvement in data retrieval. Finally, we show some interesting insights within the recently released AOL search data. We see the taxonomic searches in this data set echoing the trend towards higher taxa and vernacular queries, as seen within the TreeBASE data, thus reiterating the use of taxonomy and ontologies as key information retrieval tools.

7.4 Taxonomic Infrastructure requirements

The taxonomic queries that TreeBASE should support are as follows.

- Search terms should expand to include subordinate terms in the classification if they are higher taxa.
- Vernacular queries should be supported and expand appropriately to include the data linked to the scientific names.
- Any given query should also expand to include data associated with synonyms and out of date usage of a taxon name.

These queries are supported in TCl-Db and demonstrated below.

7.5 TreeBASE Taxon Search Log

The TreeBASE web interface can be found at the URL *www.treebase.org.* The interface allows users to conduct taxon queries, queries by a specific matrix identifier, study, or tree identifier. These queries return the number of phylogenetic studies that contain the term that was used in the search. The database structure of TreeBASE was replicated locally so that SQL queries could be performed on specific tables within TreeBASE and TCl-Db tables linked to TreeBASE. The taxon queries on TreeBASE came from a script given to us by the TreeBASE developers. The script returned all queries performed using the taxon field in the TreeBASE user interface. This query log contains the queries and the number of times these queries had been performed. The query log was loaded into a database table and given unique identifiers. The data were initially trimmed to remove trailing spaces. Duplicates were then removed and non taxon searches, such as queries based on TreeBASE identifiers, were also removed. Searches for study authors were removed by comparing the queries to the author names stored in TreeBASE. Genbank Accession number queries were also removed from the data set. The remaining 62,126 queries were then mapped to TCl-Db giving, 27,239 queries in the query log with exact matches to a taxon name in TCl-Db. These are stored in the materialized view given in query C1 in Appendix C. The queries were compared to the taxon names in TCl-Db for a second time, allowing, this time, for case insensitive matches and single letter mismatches. Including mismatches, a total of 29,035 queries were mapped to a taxon name in TCl-Db. Using these

Database Source	Mapped Queries	MappedTreeBASE taxa
Morony,Bock and Farrand Checklist	695	97
ITIS	12785	3415
ITIS	978	258
Sp2000	15990	4566
Algaebase	224	106
NCBI	17018	5545
NCBI	15893	5485
American Ornithological Union	489	44
GRIN	5044	1945
Mammal Species of the World	950	478
bird_names	261	68
Clements Check List	261	68
Sibley and Monroe Checklist	652	88

Table 7.1: Data from Appendix C, query C4. This table shows the number of taxon names, from two data sets, that map to each data source (there are two copies of NCBI and ITIS after updates). The first data set, in column 2, are the mapped queries from the TreeBASE query log. The second data set, are the taxa within TreeBASE (column 3).

mapped queries we compare the data returned in response to these queries directly against a local copy of TreeBASE, downloaded in 2006, and through our TCl-Db wrapper.

The analysis of the query logs show that users have been experiencing very poor data retrieval. Over 1/2 of the queries, 16,018 out of 27,239, do not return data in TreeBASE. Of the valid name queries posed against TreeBASE 71% do not return data (query C2, Appendix C) with 94% of the vernacular queries and 85% of the synonym queries also returning no data. Approximately 50% of the queries posed on TreeBASE are higher taxa queries (of rank genus and above) while 28% were species queries (query C3, Appendix C) see also Figure 7.1.

Table 7.1 shows how these mapped taxa in the query log correspond to the original data sources. The first column gives the data source names, the second column gives the number of taxon queries that matched a name in these data sources. The third column is the number of TreeBASE taxa that matched a name in these data sources. A comparison of the final two columns shows that many more taxa are being used as search terms in TreeBASE than exist in TreeBASE. Taking the Sibley and Monroe Checklist as an example, 652 queries have been performed while only 88 of these names exists in TreeBASE. This table highlights the importance of data coverage and shows that one database source for a taxonomically intelligent database is insufficient. For example, Sp2000 and NCBI show similar numbers (15,990 and 15,893 respectively), there is, however, very little overlap in these names, and closer inspection showed that nearly 5,000 of the NCBI matches (1/3) were not included in Sp2000.

7.5.1 Data Retrieval in TreeBASE Vs TCl-Db

We used the taxon queries in the TreeBASE search log to determine if the current taxonomic capabilities of TreeBASE could be improved with the addition of TCl-Db. Since only half of the mapped queries returned a tree in TreeBASE, we were convinced that this could be improved using TCl-Db. A comparison of the query capacity of these queries against TreeBASE and against TCl-Db linked to TreeBASE is given below.

The comparison is based on the number of trees returned by the queries. In the web interface of TreeBASE, studyids are returned. The data given here are tree counts and not study counts, and therefore are not directly reproducible on the TreeBASE web site. We found that in the version of TreeBASE we had, studyids could not be used as a stable measure of retrieval. In order to determine the number of studies returned for each taxon query, four tables need to be joined. The joins proved to be unstable since the data lacked referential integrity. However, the table TREETAXA with the key TreeID linked directly to the TAXA table which provides stable queries and an efficient and reliable measure of data retrieval. A few queries to return studies were performed to confirm and double check the results. Where available these have been shown in the data below.

The data retrieval capacity of TreeBASE for each taxon query was calculated using the query C1 in Appendix C.1. The total number of trees returned by the taxon query data set from directly searching the TreeBASE taxa table was 2,962 distinct trees (1,775 distinct matrices). The distribution of TreeBASE taxa and the TreeBASE queries by taxonomic rank is summarised in Figure 7.1 . The total higher taxa queries were calculated from subgenus and above and the species count includes subspecies and lower rank queries. The pie charts show that the majority of TreeBASE names are Species while the majority of queries performed on TreeBASE are higher taxa names. Table 7.2 shows more detail by rank, of the TreeBASE taxon query log. The percentage of queries of Species and lower ranks is 30%, for higher taxa 50%, and 38% for NULL rank values (rank data was not available). The reason these numbers do not add up to 100 is due to duplicated taxon names across ranks and differences in ranking between data sources. Some examples of this are shown in the last column of Table 7.2 where taxa are included in more than one rank, due to differences in classification across the data sources as highlighted in bold. With the exception of a few examples in Genus and Subgenus, this was more prevalent in the ranks above Family. There are instances where some data sources did not give rank data for particular names but the rank was available from other data sources, e.g. Myxomycota, Oomycota. In the ranks Class and Subclass there are examples of different forms of the same taxon name, spelt differently e.g., (Granuloreticulosa, Granuloreticulosea) and (Hamamelidae, Hamamelididae). From this data we are able to conclude that the poor data retrieval is due to use of names that are not contained within TreeBASE. Since TreeBASE does not contain a hierarchy, and majority of the queries are higher taxa, it is not surprising that data retrieval rate shown in the query log is so poor.

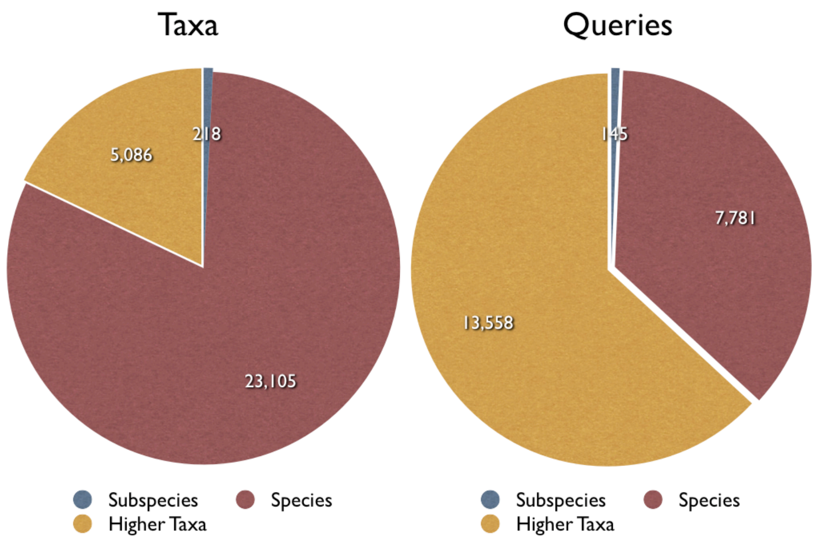


Figure 7.1: TreeBASE taxon content and the TreeBASE taxon query log. The difference between the distribution of taxon names in TreeBASE and the TreeBASE query log is large. The vast majority of taxa in TreeBASE are species (left) while the types of queries performed on TreeBASE concern higher taxa. (From query C3 given in Appendix C)

7.5.1.1 TCl-Db linked names improve data retrieval.

Poor data retrieval, like poor communication, is the result of lack of understanding. The queries do not return data because the query term is not understood by the database. One way to improve this is by increasing 'the vocabulary' of the database. The addition of a taxonomy into the TreeBASE structure would enable the queries to be understood by the system and make it more user friendly. With the majority of queries not returning data through a direct search on TreeBASE, we performed these queries through TCl-Db in-order to compare the retrieval capacity of the search terms through a more complete taxonomic data source.

Synonym queries

Count (Taxon Names)	**Rank**	**%(of 27239)**	
7781	Species	28%	
145	Subspecies		
20	Infraspecies		
105	Tribe		
9	Subtribe		
137	Variety		
15	Varietas		
1	species subgroup		
8213	Total Species and lower ranks	**30%**	

Count (Taxon Names)	**Rank**	**%(of 27239)**	**Examples**
8	Superkingdom		Eucarya, Eukarya, Eukaryotae, eukaryotes
21	Kingdom		**Chromista**, Metazoa, Fungi
3	Subkingdom		**Chromista**, Tracheobionta
11	Superclass		Gnathostomata, Osteichthyes
279	Class	1%	**Ophiuroidea, Monogenea** Granuloreticulosa, Granuloreticulosea
90	Subclass		**Ophiuroidea, Monogenea** Hamamelidae, Hamamelididae
14	Infraclass		Eutheria, Holometabola, Endopterygota, Dipnoi
1	Superphylum		
203	Phylum		Protozoa, Rhodophyta, Chordata **Oomycota, Myxomycota**
30	Subphylum		Pezizomycotina, Pentastoma, Myriapoda, Mycetozoa
40	Superorder		**Salientia, Parasitiformes**, Palaeognathae, Neognathae
683	Order	2.4%	Neogastropoda, Galliformes **Salientia,Parasitiformes**
142	Suborder		**Strongylida**, Iguania **Tylenchida, Symphyta**
33	Infraorder		Stratiomyomorpha, Palinura,
3	Parvorder		Amphisbaenia, Heteroneura,
81	Superfamily		Tylenchoidea, Scorpionoidea,
1767	Family	7.3%	**Crocodylidae**, Hominidae **Viperinae, Sphinginae**
208	Subfamily	0.9%	**Crocodylidae**, Alligatorinae
9971	Genus	37%	*Solea ,Fusobacterium, Parvovirus, Anopheles*
45	Subgenus		Sarcophaga,Pelophylax, **Xenopus,Pinus,Anopheles**
202	no rank		Coelomata,Amniota,Anopheles *Escherichia coli K12, Fusarium solani* **Myxomycota**,Myxomycetes,**Oomycota**
13835	Total Higher taxa	**50%**	

Count (Taxon Names)	**Rank**	**%(of 27239)**	**Included Names**
10512	NULL	**38%**	Catherpes,Corvus, Oenothera, Dragon, Lemna minor

Table 7.2: Distribution by rank of TreeBASE Taxon Queries. (From query C3 in Appendix C.)

In the TreeBASE query log we found that 85% of the queries that were synonyms returned no data. Expanding search terms in TCl-Db improves data retrieval for synonym queries. The 868 synonym queries that returned no data in TreeBASE alone, returned 594 trees when TCl-Db was used. These queries used the query expansion within TCL-Db. Valid names are linked to synonyms, so that when a query is performed using a synonym, TCl-Db is able to use the

Query	TCl-Db Query	TCl-Db retrieval	TreeBASE retrieval
maple	Acer	7	0
primates	primata	3	2
pine	*Pinus brutia*	2	0
pine	Pinus	7	0
eubacteria	Bacteria	2	0
mouse	*Mus musculus*	28	0
birds	Aves	8	0
dog	*Canis familiaris*	19	0
mammals	Mammalia	12	0
human	*Homo sapiens*	52	0
elm	Ulmus	2	0
Acacia	*Parkinsonia aculeata*	2	0
Acacia	*Acacia ampliceps*	2	0
Acacia	*Robinia pseudoacacia*	10	0
yeast	*Saccharomyces cerevisiae*	70	0

Table 7.3: The most common vernacular queries with Latin names and the number of trees found for each query. (Appendix C, query C5)

linked name as part of the search.

Vernacular queries

Vernacular queries on TreeBASE perform particularly poorly. While these are not the most frequently used search terms, TCl-Db allows these terms to expand to Latin names. The retrieval for vernacular queries is exemplified in Table 7.3. The vernacular 'acacia' translates to *Robinia pseudoacacia*. Using the search term acacia returns no data in TreeBASE while the Latin term, related to acacia, returns 2 trees. In TCl-Db, the inclusion of the alternative Latin names improves the quality of data retrieval. For those queries that translate to higher taxa names, data retrieval can be further enhanced by performing a hierarchical query.

With higher taxa queries we would expect a significant improvement when the queries translate to include all subordinate taxa (since more names are included in the search). Further, since most of the queries performed were higher taxa names, it is important to quantify the expected increase.

7.5.1.2 TCl-Db hierarchical queries show superior data retrieval.

Hierarchical queries are those where the search term is a higher taxon name and the query expands to include all names subordinate to it. With a family name, for example, the query would search the family name, all genera, and all species considered within the family. Tables 7.4 and 7.5 show a comparison of query effectiveness of TreeBASE alone and TCl-Db used in conjunction with TreeBASE. The most significant improvement in the quality of data retrieval is seen for 'pinus' (Table 7.4) and 'Metazoa' (Table 7.5).

Using the 6622 generic queries that return no data in TreeBASE, these queries were re-run using TCl-Db. A total of 1,127 trees are returned when hierarchical query expansion is used. If a query is translated to include all terms below it in a hierarchy, we can assume that the search will return far more data than a simple name search with only one term. For example, the query term *Aspergillus* expands from one term to 155, returning 38 more trees than the term *Aspergillus* alone (more examples in Table 7.4). If we assume that this is what the user meant when he performed the query, then many more data can be returned when expanding the search term hierarchically. One caveat to consider here is which classification to use when performing this type of query. The *Aspergillus* query was expanded using the NCBI classification which from previous data we know to have good data coverage for Bacteria and Fungi. The same query using ITIS returns no species because the genus does not exist in ITIS. In this scenario, where one database contains data and where the other does not, the decision is straight-forward. However, given the situation where the term exists in both databases but the distribution of species names were different, which one should be used? The combined data in TCl-Db enables us to perform such a query through multiple hierarchies returning all unique names. It would be pertinent for the user to be told exactly which names were included in the search, so that he could exclude those he wished to use. When the *Aspergillus* query is repeated for all unique names subordinate to Aspergillus, without specifying the source database, the species number expands to 262, which returns 43 trees (Table 7.4).

The genus rank provides a very simple and efficient query in the TCl-Db data structure, (see Appendix C, Queries C6 and C7). Table 7.4 shows considerable improvement in data retrieval when the query expands to include species within a Genus search. Higher taxa queries above the Genus rank are more complicated to perform, and an example is given in Appendix C, query C8. The table highlights the importance of including more than one hierarchy. For instance, the query 'Metazoa' returns no data when using the ITIS or Sp2000, but over 1000 trees in NCBI. Similarly, for 'Fungi' we see that NCBI and ITIS differ considerably. In some cases the hierarchical query failed, and this is denoted with an **X**. For example, the term 'Archaea' is both a genus and superkingdom in SP2K, causing the hierarchical query to fail (see Section 8.3). Initially the queries producing data given in Table 7.5, were performed individually, for each data source. To make these higher taxa queries more efficient, a materialized view was created to capture data from the NODE table and the mapped names. Using this view, a subsequent view was created in which the hierarchical queries are pre-calculated for each of the mapped names for the SP2K, NCBI and ITIS classifications.

Genus	ITIS species count	NCBI species count	Sp2000 species count	Trees Returned from TreeBASE	Additional Trees Returned Using TCl-Db
Platanus	6	5	6	23	2
Drosophila	**378**	**43**	**2066**	**28**	**88**
Saccharomyces	13	62	6	26	73
Homo	1	1	1	1	52
Quercus	214	89	211	1	5
Pinus	**62**	**66**	**57**	**7**	**123**
Arabidopsis	2	10	2	9	37
Acer	21	79	21	7	9
Canis	7	10	7	9	29
Pan	2	2	2	1	4
Escherichia	21	1	7	0	8
Acacia	62	160	1315	0	4
Acorus	2	4	2	13	1
Phytophthora	1	74	58	13	29
Mus	38	25	38	28	30
Bacillus	1	1450	150	1	5
Magnolia	12	76	134	8	4
Aspergillus	0	155	185	5	43
Fusarium	0	183	85	2	19
Tetragnatha	0	21	323	6	6

Table 7.4: The number of species within each genus for ITIS, NCBI and Sp2000. Each source shows varied species content for each genus, e.g. *Pinus* and *Drosophila*. The last two columns show the number of trees returned for the genus in TreeBASE; and the number of additional trees returned using species names from hierarchical query expansion in TCl-Db. This table was populated using the query exemplified in C7, Appendix C

7.6 AOL Search queries

America Online (www.AOL.com) is a large search and internet provider in the USA. AOL released a data set of 20 million web queries from 650,000 users, for research purposes. The data taken over a three month period includes not only the query but also the results that were clicked (referrals). We analysed this data set for taxonomy searches, to see how many and what kind of taxonomic searches were being performed in general purpose search engines. The aim was to see if higher taxa queries predominated, as was seen in the TreeBASE logs. Figure 7.2 shows that, although there are significantly more species queries on TreeBASE, the higher taxa searches within AOL search engine do indeed echo the search pattern seen in TreeBASE. As expected, given the AOL user community, vernaculars were more common searches than scientific names.

The AOL query data was loaded into a table, then sorted alphabetically, and duplicates were removed. A query to determine exact matches to names in TCl-Db was run first. These matches were counted and removed and the remaining data was compared to a dictionary to remove English words. The remainder of the data set was then compared to a list of taxon names extracted from TCl-Db using Agrep, allowing for one mismatch. A second iteration with Agrep using two mismatches was also performed but discarded, as the shorter queries returned

	Number of Trees Returned Using:			
QUERY	TreeBASE	Sp2000 Hierarchy	ITIS Hierarchy	NCBI Hierarchy
Diptera	7	X	111	106
Lepidoptera	5	41	39	71
Carnivora	12	49	49	65
Animalia	1	954	856	0
Solanaceae	9	80	80	80
Rosaceae	1	42	42	38
Felidae	7	10	10	15
Vertebrata	3	0	408	443
Fungi	**8**	**807**	**389**	**814**
Crustacea	2	0	47	38
Chordata	1	433	411	446
Metazoa	**5**	**0**	**0**	**1014**
Poaceae	11	100	100	95
Rodentia	9	100	100	102
Chlorophyceae	6	50	66	50
Cnidaria	3	75	78	79
Arthropoda	5	404	284	371
Primates	7	61	61	61
Aves	8	91	91	87
Reptilia	1	74	74	0
Coleoptera	3	67	45	49
Cetacea	16	47	17	47
Bacteria	2	55	13	35
Ascomycota	9	549	273	540
Archaea	**4**	**X**	**0**	**15**
Mollusca	14	75	86	93
Mammalia	12	224	212	221
Fabaceae	11	151	143	151
Asteraceae	11	127	127	156
Insecta	2	325	238	301

Table 7.5: Expanding query terms hierarchically increases the number of trees returned from TreeBASE. The first column shows the number of tree returned from TreeBASE. The remaining columns show the number of trees returned using hierarchical query expansion using classifications in TCl-Db. This table was populated using the query example given in C8, Appendix C

too many matches to usefully determine the actual query. The exact matches and the Agrep single letter mismatches were loaded into a table and examined in detail.

This data set contained 8,281 taxonomic queries, of which 3,590 were vernacular names, 367 were synonyms and 3,076 were valid names. When the data were compared allowing for misspellings, these figures increased. With a mismatch of one for queries greater than four characters in length, we first selected the approximate matches that have only one Agrep hit, which gave 1708 additional queries mapped to a taxonomic name.

However, there were far more Agrep matches that could not be included in the analysis. When using a mismatch of one or two, especially with the shorter queries, we could not be sure that the hit given by Agrep was what the user was requesting. With the TreeBASE query data we were more confident that the Agrep match was a taxon name. However, the AOL search data can not be treated the same way as the TreeBASE query log, since the TreeBASE log was based on taxon searches. For example, the Agrep match of Ortegon to the query Oregon could

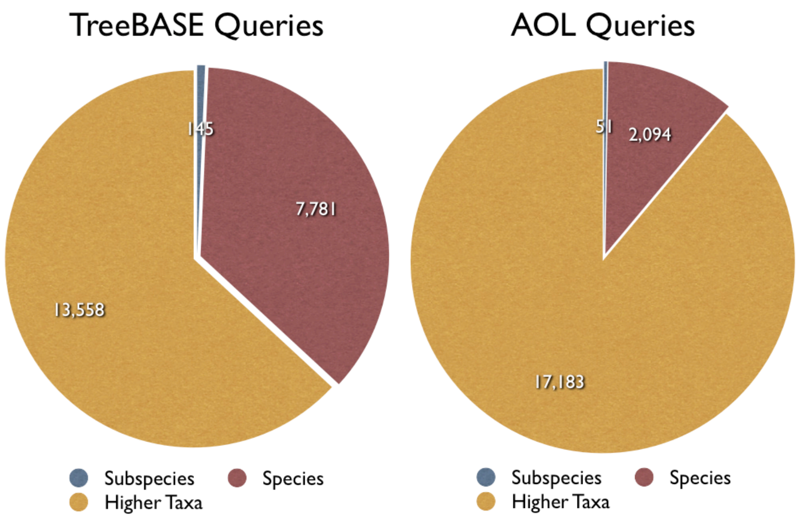


Figure 7.2: TreeBASE query log and the AOL query log. Given a similar number of queries, there are roughly three times as many species queries in TreeBASE as in AOL.

be misleading; the same is true for Volvo matching the query term Volva, and other examples. Where two or more Agrep matches were found for a query, we had to check each referral to pick the Agrep match that was the actual query the user was placing. This was too large a task, considering the size of the data set (265,909 Agrep matches). Instead, we looked only at the exact matches that were found in the AOL log and the single letter mismatches that had only one Agrep match.

The AOL Taxon queries are summarised by rank in Table 7.6. Some of the data in the higher ranks were manually checked through referrals. The 3 superkingdoms searched were ARCHAEA, BACTERIA AND EUKARYOTE. Ten Kingdom searches were placed but no referrals were made from these searches. However, considering the unique nature of these terms, there is little ambiguity in the users' intentions. Out of 44 Phylum searches, 34 had referrals. The most common taxon search term was CHLAMYDIA, with 202 searches, however, the majority of referrals were for various sexual health sites and only one referral was made to NCBI.

There were 6 queries that approximately matched to taxon in the rank Class. Those verified as taxon queries were GASTROPODS (three searches), TRICHOMONADS (one search - no referral), CEPHALPODS (four searches), NUSA (one search - no referral), and RUDA. In Subclass, there were five approximate matches and all but one search had a referral. In the Superorder, all but

Rank	AOL Query Count
Superkingdom	2
Kingdom	7
Phylum	44
Superclass	1
Class	48
Subclass	12
Superorder	2
Order	82
Superfamily	4
Family	208
Subfamily	8
Genus	2658
Subgenus	9
Species	1870
Subspecies	47
Infraspecies	5
Variety	51
Tribe	1

Table 7.6: Referral URLs from the AOL Log. Each URL was searched against the AOL data using http://www.seosleuth.com/site/.

one of the three searches were valid taxon queries. Since there were 185 searches in the Order rank, we verified only the valid names that were approximate matches, making the assumption that the others are true taxon searches. In this set there were 7 searches, one of which turned out to be a car search performed 391 times, ACURA. The next most abundant search from this group was SPIRULINA, with 47 searches.

The referral data was the more interesting and useful part of the AOL queries. We were able to check the number of referrals made to various taxonomic name servers including ITIS, NCBI, uBio and Sp2000. The servers within Sp2000(www.catalogueoflife.org) and UBio had no referrals from taxonomic name searches, while ITIS and NCBI did. Taking into account the search terms used and the technology used by name servers in comparison to systems like tolweb.org that serve simple (botable) html pages, this is perhaps not a huge surprise. However, considering the enormous amount of taxonomic data available on the web, the AOL data shows that not much of it is being searched for or indeed being found by the general public. Considering this, it may be appropriate for projects such as the Encyclopaedia of life (EOL, 2008) to make their species pages discoverable via general purpose search engines such as AOL and Google (see section 8.3).

Referral URL	Total No. of Searches	Total Unique Keywords referred
www.itis.usda.gov	36	28
www.ubio.org	0	0
ubio.mbl.edu	0	0
www.ncbi.nlm.nih.gov	16180	12674
darwin.zoology.gla.ac.uk	9	8
www.otlweb.org	4	4
www.ipni.org	7	6
www.indexfungorum.org	3	3
www.mbl.edu	26	22
www.catalogueoflife	0	0
www.sp2000.org	2	2
www.gbif.org	0	0

Table 7.7: Referral URLs from the AOL Log. Each URL was searched against the AOL data using http://www.seosleuth.com/site/.

7.7 Discussion

We have shown that the inclusion of TCl-Db data makes a significant impact on information retrieval by linking vernaculars and higher taxa queries to their related terms. As stated, one explanation for the queries returning no data is the taxon content of TreeBASE, as there is no data to retrieve for these names. For example, given that most TreeBASE taxa are valid species names, it is not surprising that vernacular names return little data. Through TCl-Db, however, the vernacular queries that did not return data were extended to include linked valid names, resulting in the retrieval of 868 trees (426 matrices). Similarly, for the synonym queries that were returning no data, queries routed through TCl-Db's linked names returned 594 trees (252 matrices). Also, for the valid names that returned no TreeBASE data we performed a hierarchical query for 6,622 genera, returning 1,127 trees (671 matrices). Therefore, using TCl-Db we can retrieve more data from TreeBASE using search terms that are not contained within TreeBASE.

There were a significant number of queries that mapped to a name in TCl-Db but did not return data in TreeBASE. 16,018 were valid taxon queries (queries mapped to a name TCl-Db) and did not retrieve data in TreeBASE. This is because the vast majority of queries posed on TreeBASE are higher taxa terms that are not contained in any trees within TreeBASE.

The analysis above shows that TreeBASE displays both poor data retrieval and poor information retrieval. From 62,126 queries, 2,962 trees are returned, giving a 4.7% data retrieval rate. From the complete query log, 27,239 queries were mapped to taxa in TCl-Db, returning a total number of 2,748 trees with a higher retrieval rate of 10.8%. While the ratio of data retrieval from the mapped names is better, the actual numbers of trees returned are similar.

This is because both data sets are searched through the same data content, i.e. the TAXA table in TreeBASE. The poor data retrieval rate is therefore a property of the taxonomic content of TreeBASE, specifically, the limited taxonomic content of TreeBASE and the fact that most of the queries posed are not names contained in TreeBASE.

The taxonomic data content in the version of TreeBASE used was 56,712 taxa. As stated above, 27,239 mapped to a name in the TCl-Db database and 31,459 were extensively mapped by Page (2007), using a number of data sources including uBio. Over 25,000 taxa in TreeBASE can not be mapped to an online taxonomic data source. These figures suggest that the Taxon content of TreeBASE is of poor quality, and the mapping performed showed that not all the data labelled as taxon names are in fact proper taxon names. Including TCl-Db taxa into TreeBASE did show a substantial increase in data retrieval (from 4.7% to 10.8%). However, part of the problem is also the taxon content of TreeBASE, and cleaning the taxa data in TreeBASE would significantly improve the data retrieval further.

While the improvements described above could be achieved using any taxonomy database, the multiple data sources and the storage of more than one hierarchy in TCl-Db is an important factor in terms of data coverage as shown in Table 7.2. The number of queries that mapped to a taxon in TCl-Db were 27,239. The distribution of these across the data sources in TCl-Db is shown in column 2 of Table 7.1. Although there is a significant overlap in the taxa across the data sources, NCBI and Sp2000 show the best coverage. Similarly, the taxon content of TreeBASE mapped to the TCl-Db data sources shows NCBI and Sp2000 fairing almost equally. However, the classification differences between Sp2000 and NCBI are significant, and picking one over the other would impair some users. Table 7.4 also highlights the data distribution in genera across ITIS, NCBI and Sp2000. The most commonly performed genus queries are given in the first column and the number of children within each data source is given in columns 2, 3 and 4. The last two columns show the substantial improvement in data retrieval achieved by using TCl-Db. Also, Table 7.5 shows the data retrieval of the most frequent higher taxon queries across different hierarchies. ITIS and Sp2000 performed similarly in most cases. Aves and Fungi are the most notable exceptions and highlights the effect of the differences in taxonomic content of the different databases.

7.8 Conclusions

TreeBASE is an example of a data set that has not been equipped with complete metadata, rendering the retrieval of data difficult and cumbersome. The data retrieval capacity afforded by the inclusion of metadata such as ontologies and taxonomies is well established in this thesis. Given that taxonomic names are such an integral part of this data, it is inexcusable not to force the inclusion of taxonomy, especially now, with the technology and databases currently available. The analysis here shows the importance of taxonomic data for more efficient data retrieval in TreeBASE and the use of an amalgamated taxonomy data warehouse to accommodate coverage and differing opinions in taxonomy. The TCl-Db warehouse provides an infrastructure to support effective data retrieval from TreeBASE. An application has been built to wrap taxon queries through TreeBASE was described in Chapter 5. The wrapper returns the expected treeids and matrixids which are linked directly to the TreeBASE website for the user to continue their download.

Chapter 8

Discussion and Conclusion

We have shown in the previous Chapter that TCl-Db improves data retrieval through TreeBASE, corroborating the hypothesis given in Chapter 1. In this Chapter, we revisit the original requirements that were laid out and address the contribution that TCl-Db has made in context of other work in this area. This Chapter concludes with a discussion of an alternative method that, in future, could be used to address data integration more economically and finally, further work and improvements that have been highlighted through the course of writing this thesis.

8.1 Overview

This research project aimed to address the taxonomic requirements of the systematics community and was motivated by the inadequate taxonomic data retrieval in TreeBASE. A data warehouse solution to this problem, TCl-Db, the Taxonomy and Classification Database, addresses the taxonomic requirements of TreeBASE. The data structure is described in Chapter 3, and Chapter 4 gives an overview of the data that contribute to the warehouse and how these were loaded into the integrated TCl-Db schema. Queries enabled by TCl-Db are described and web tools that were built to use TCl-Db are presented in Chapter 5. TCl-Db provides breadth of coverage by integrating multiple taxonomic data sources. As shown in Chapter 6, there are significant differences in the data held by different data sources. Chapter 6 also highlighted the classification differences that required TCl-Db to store and deliver hierarchical queries through a choice of classifications. In Chapter 7 we demonstrated the improved data retrieval that can be achieved by including a taxonomic infrastructure within TreeBASE. This Chapter highlighted the use of query expansion for higher taxa, synonyms and vernaculars that significantly improved data retrieval. This current chapter discusses this work and an alternative technology that can be used in the future developments of TCl-Db.

8.2 Contribution

TCl-Db was designed for two specific types of consumers: those who require access to data through taxon name queries in TreeBASE and those who gather data from multiple sources where names need to be reconciled before analysis, for example in a supertree analysis. The first requirement was delivered and demonstrated in Chapter 7 and the second was demonstrated in Chapter 6. These requirements are now also being addressed by the wider community and will eventually be superseded by TreeBASEII and Global Taxonomic Initiative and its partners. For the time being, these requirements are met by TCl-Db.

The core of TCl-Db development consisted of data integration. Data integration addresses several aspects of taxonomic data that cause difficulty in the user community. Integrated taxonomic data increases accessibility of disparate data, as data redundancy is reduced by combining data from several sources into a single structure, and combined data can be compared to highlight differences and discrepancies. In Chapter 6 we showed how the data sources used in TCl-Db can be compared side by side. In Section 5.3 we presented SQL queries which identify homonyms, differences in name usage (synonyms and valid names) across the data sources and classification differences between data sources (Section 5.3.1).

These analysis queries were extended in Chapter 6 and used to add data to TCl-Db. The integrated data were used to make complete the information, through the addition of, for example, rank information to data sources that did not hold these data. Additional linked names were generated via the identification of spelling differences, and queries were formulated that easily map names to different classifications (Table 6.7). In Chapter 6 we were also able to corroborate links that were created through usage differences. For example, in Chapter 5 we showed that Casuariidae and Dromaiidae were linked as synonyms. The comparison of NCBI and ITIS alone could not corroborate this link, however, the addition of Aves check lists enable this link to be validated. Queries to corroborate the links that are created in TCl-Db are easy to specify, since the original data sources are linked in to the global TCl-Db schema.

The integrated data in TCl-Db are used as a taxonomic infrastructure for TreeBASE. In Chapter 7 we demonstrated significantly improved data retrieval using taxonomic queries through TCl-Db linked to TreeBASE. TCl-Db enables query expansion of higher taxa query terms, synonym and vernacular query terms and provides breadth of taxonomic coverage.

The user requirements laid out in Chapter 1 have been met and demonstrated through this work. Several aspects were highlighted for improvement through the course of writing this thesis, particularly, aspects of the data model and the user interface that can be improved. An alternative method that is increasingly being used in the taxonomic and biodiversity community are semantic web technologies. These technologies were briefly explored and an evaluation exercise highlighted their potential use in the future developments of TCl-Db. This chapter continues with a listing of further work proposed from these discussions.

8.3 Discussion

8.3.1 Related Work

The motivation for developing TCl-Db was to deliver a taxonomic infrastructure that could be used with TreeBASE. The current version of TreeBASE is soon to be replaced by Cyberinfrastructure for Phylogenetic Research (CIPRES) TreeBASEII (CIPRES, 2006). A prototype was due for release in July 2006 but is not yet available. The new improved TreeBASE schema has been published (CIPRES, 2006) and contains a Taxon module which looks to rectify many of the data retrieval issues currently experienced by users. At this stage, with only architecture and structural documentation, it is difficult to see exactly how hierarchical and vernacular queries will be supported in TreeBASEII.

The schema contains a taxon module describing the objects TaxonLabel, TaxonLabelSet, Taxon, TaxonSet, TaxonLink and others. The documentation states that the Taxon object holds a unique taxon name. Through the TaxonLink this will connect users to an external taxon authority. The TaxonAuthority object makes reference to NCBI, uBio and SEEK, as examples. TreeBASEII also plans to make use of LSIDs (Life Science IDentifiers (Miranker *et al.*, 2008)) as a mode of unique identification and information integration with other data authorities. Creating these links will also require extensive data mappings of each TreeBASE taxon to taxa names in each data authority, similar to the exercise performed in this research for TreeBASE names in Chapter 6. Without actually testing the prototype it is difficult to tell if this new improved data structure will support the queries users are performing on the current version of TreeBASE. Until the TreeBASEII system comes online, TCl-Db offers a solution that enables more effective data retrieval using taxon names, as demonstrated in Chapter 7.

Attaching a taxonomic infrastructure to TreeBASE can be achieved in a number of ways.

A recent solution was provided by Phylofinder (Duhong *et al.*, 2008). Phylofinder offers a taxonomic backbone to TreeBASE via TBmap and the NCBI classification. The solution offered by TCl-Db is superior to the simple approach used in Phylofinder. A comparison of TreeBASE queries using Phylofinder and TCl-Db shows that while Phylofinder does indeed improve data retrieval, it has some severe limitations resulting from using only one classification. Higher taxa queries from the ITIS classification that are not used in NCBI, or that have not been mapped in TBmap fail to return data. TCl-Db does not have this limitation, since TCl-Db contains full classifications and TreeBASE mappings to ITIS and other resources. TBmap will also expire with time, while the mappings to TreeBASE made via TCl-Db can be maintained very efficiently with SQL queries that can be rerun after each new update

uBio has a very similar scope and remit to TCl-Db, however, it is only available through web services, which means that their data can not be physically integrated into TreeBASE. The performance of SOAP services provided by uBio could be severely limiting. Performance of web service mediated data queries does not compare to queries performed through physical integration, and this was one of the reasons that we choose a data warehouse approach.

Since this project used data integration in order to deliver data coverage, and data transformation was required to deliver hierarchical queries, a data warehouse within the relational data model was deemed to be the most appropriate method.

TreeBASE, and most of the other taxonomic databases, are built using relational database technology. Technologies developed by the W3C for the semantic web have been highlighted as an alternative solution for data integration. This alternative method was briefly explored (see Appendix D), since it offers to deliver all the advantages offered by a data warehouse without replicating data within a warehouse and the technologies offer a mediated solution that would be far easier to maintain than traditional web mediated services.

8.3.2 Semantic Data Integration

From a database perspective, data integration assembles data from several data silos and maps those into a shared schema. Integration is achieved by applying queries on this schema. On the web, data are not integrated but are linked together using URLs. This is achieved through the addition of A HREF tags around URLs within documents marked up in HTML or XHTML. These tags enable a user to browse from the current data to relevant data, as linked by the author. Using semantic web technologies (Berners-Lee & Hendler, 2001) resources on the web, given correct metadata (Resnik, 1995), new resources can be discovered which would remove the need for human mediated links. With the addition of metadata, the resources become semantically rich and have meaning to computers as well as the users browsing them (Amann *et al.*, 2000). Since computers have the capacity to use the metadata, data discovery on the web can be made possible.

Data integration was highlighted as one of the core uses of semantic web technologies (Heflin & Hendler, 2001). Making taxonomic data interoperable across the web (Williams, 1997) would be of great benefit, considering the investments made so far and also the distributed nature of the science. The potential use of the semantic web (Berners-Lee *et al.*, 2001b) for data integration is now well acknowledged and solutions are being implemented in several areas of life sciences (Good & Wilkinson, 2006; Stevens *et al.*, 2006) of which, the taxonomic community has also taken note of these developments (Page, 2007).

The semantic web uses several layers of technology (W.3.C., 2006). When these are used together, they add increasingly richer expressivity to data (via metadata). In the bottom layer a global naming scheme, through URI's is required. A URI, Uniform Resource Identifier, is simply a web identifier and any data object in the semantic model must have a unique URI. Currently GUIDs [1] and LSIDs [2] are being tested as solutions within the biodiversity community (Page, 2008). Above this layer is XML and XML Schema. These languages have been in use for many years already. XML adds surface syntax to data and XML schema is used to describe the structure of data in an XML document. The taxonomic community has invested in this area also through the adoption of a data exchange format in XML (Kennedy, 2005) and controlled vocabularies such as Darwin Core for geographic occurrence and specimen information. Layered over XML and XML-S, is the core semantic web technology technology, RDF, the Resource Description Framework (http://www.w3.org/RDF/).

RDF provides a standard syntax for describing data and is the layer at which data can be brought together. RDF provides a consistent standardised way to describe and query resources with syntactic interoperability. In essence, RDF is a data model that describes relationships between things, web resources, data elements, or objects. Data in RDF are represented as triples: a subject (with a unique URI), a relation (the predicate) that describes the relationship to an object or data value. In RDF, data are annotated with metadata in a machine readable way though these relations (or properties). To enable interoperability a common shared vocabulary is required and this is provided via RDF-Schema, an RDF vocabulary dictionary. RDF is also

[1] Globally Unique Identifier

[2] Life Science Identifier

being adopted. IPNI offers their data in RDF and uBio offers a tool (http://www.ubio.org/rss/) that can collect taxonomic names from data provided by the RSS [1] feeds from publishers of scientific literature.

The Web Ontology language, OWL, adds even more expressiveness to the data. So far, not much progress has been made in this area, but this is undoubtedly where future investment will be focused, as current efforts progress and the base layers described above are in place. The Biodiversity community are making significant strides towards delivering and using data from these technologies. The Encyclopaedia of Life (Wilson, 2003) is one project following the semantic web ethos (Saaed *et al.*, 2008).

With Oracle providing support for RDF within the Oracle spatial product, we were able to get a feel for this technology by using the integrated data in TCl-Db and a local copy of TreeBASE (see Appendix D). Several observations were made while this technology was tested. These are as follows.

- Conversion from relational data into RDF is fairly simple and several tools exist that support this (Bizer, 2003). Serialising RDF using SQLX was trivial, and XSLT scripts also took very little time and effort to write. The N3 notation (Berners-Lee, 1998) is much more user friendly and easier to handle than the RDF/XML format (Beckett *et al.*, 2003).

- Queries were very intuitive, following SQL and SPARQL like syntax, but more complex queries required an intimate understanding of the graph structure where a visualisation of the graph would have been useful. Oracle provides the ability to query data in the RDF network and relational tables together through SQL which was incredibly powerful.

- On the whole, the experiences gained were very useful and it is clear that this has the potential to be a more cost effective integration technology.

- From this small exercise we conducted, performance and scalability are still limiting.

- Systems that have fully adopted the semantic web ethos are still few and far between and it will be sometime before the advantages are fully realised.

- We do see the advantages offered by the semantic web and TCl-Db will in the future move towards delivering data that can be used and discovered automatically. The web services

[1] RDF Site Summary

described in Chapter 5 go some way to provide this already and this will be extended and progressed.

The experiences gained from testing these technologies allowed us to develop ideas for future developments and additions to TCl-Db.

8.3.3 RSS Feeds and Data Update

One of the biggest challenges in a data warehouse system is maintenance and keeping data up to date. Currently, data refresh is manual and laborious, though it could be automated using database triggers. This was touched upon in section 4.7 and was attempted. However, only NCBI's data worked through this mechanism. The ITIS and Sp2000 updates had to be performed manually. As more data sources move toward providing their data in RDF via RSS feeds, the possibilities for maintenance and data update through these data feeds will enable the data in the system to be more easily kept up to date.

RSS, RDF Site Summary, is already used to aggregate content form multiple web resources (Hammond *et al.*, 2004). Google news, for example, uses RSS feeds from various news sources and aggregates the contents into a single page. As mentioned above, this technology is also being used by uBio to gather new names that are published in the scientific literature (Leary *et al.*, 2007). In the same way that these applications gather data, TCl-Db can use RSS feeds to collect data from databases that publish updates through RSS. Currently, few database provide updates to their data sources in this manner, however, NCBI are moving in this direction (Sahoo *et al.*, 2007) and it will not be long before this becomes a more popular method of content delivery.

To this end, the future development will primarily focus on maintaining TCl-Db data in RDF. In the proposed architecture, the assertion data in TCl-Db would be stored as a single RDF graph. New assertions can easily be added. This requires the data sources to set up an RSS feed, and the data in the feeds can then be automatically sent to a software client that converts the assertions into the TCl-Db RDF graph. This would be one mechanism that could keep assertions up to date within the database. However, this would only work well for lower taxa, where there is no impact on the source classification. Higher taxa names that are changed or added from the sources would require a full update in order to build the nested set and materialised path data. Additionally, by maintaining the assertion data in RDF, these data can be syndicated to other aggregators or resources on the web.

8.3.4 The Data Model

There are two aspects of the TCl-Db data model that could be improved in the future. Since these did not affect the function of TCl-Db significantly, they were not implemented, however, these improvements could enable further uses of the TCl-Db data by databases other than TreeBASE. These improvements concern the way the database stores synonyms and their provenance and the implementation of hierarchical queries.

Synonyms are stored in the database through the use of the name_status attribute in the NAME table. The placement of name_status in the ASSERTION table would have been more appropriate. The placement of name_status in the name table may result in data loss during transformation. Since different databases treat taxonomic names differently, there were many situations where names considered valid in some databases and considered synonyms in others. Therefore, by attaching name_status as an attribute of NAME, we lose the different status opinions from other databases databases and fail to preserve data provenance Buneman *et al.* (2000).

As ITIS was the first data source loaded, the names from ITIS were the first to fill the attributes in NAME. During subsequent data loads from NCBI and other data sources, the status of the name, if it was already in the database came from ITIS , and if the status was different from that recorded in ITIS this data would be lost. When this was observed, a simple solution was put in place. Since we maintained each copy of the data sources in individual data silos, we were able to gather this data by querying individual silos. These data are stored in a materialised view, however, this is not a permanent fix and the model should be adjusted in future work to enable name status from the different data sources to be maintained in the data model. Since this had no effect on querying TreeBASE, it was not deemed important to change, but this does limit other uses of TCl-Db and therefore will be addressed in future versions.

Homonyms caused problems with hierarchical queries using Oracle's CONNECT BY utility. There were several situations where a single name is placed in several ranks within the same database. Examples mentioned in previous chapters are: Drosophila which in NCBI is in the rank Genus and the rank subgenus and Archaea in Sp2000, which is both a kingdom and a genus in the Animalia kingdom. While performing the data analysis queries described in Chapter 5, it was discovered that the homonyms in hierarchical queries would fail. In the TCl-Db data model, homonyms have the same name_id but different parent_name_ids in the NODE table, and having a name_id in the tree twice creates a loop in the CONNECT BY query. One resolution to this would be to use an assertion_id and parent_assertion_id in place of name_id and parent_name_id. Alternatively, a more robust solution would be to identify homonyms during the data load procedures and give them unique identifiers. Since alternative hierarchical queries, using the materialised paths and nested sets still work, and these are used by the web tools, a short term fix was not necessary in this case and was not applied.

8.3.5 The User Interface

An ancestor taxa search is not currently available in the web tools described in Chapter 5. An ancestor query is equivalent to travelling up a tree. Currently, the hierarchical queries provided by TCl-Db only provide a descendant query, i.e. travelling down a tree to leaf nodes. It may be useful to provide a mechanism to go up the tree also. This query could easily be implemented within the current data model, as Oracle provides a mechanism to go up through parents using the CONNECT BY utility. For example, a query starting at Chordata and traversing up the tree would look as follows:

```
select node_id
from whouse.node
where tree_id = get_tree_id(ITIS)
start with (name_id = get_name_id(Chordata) and tree_id = get_tree_id(ITIS))
connect by prior parent_name_id = name_id
```

The nested sets work intuitively when traversing down a tree, however, ancestor relationships are hard to calculate efficiently. Materialised paths can be used instead. Traversing up a tree requires simply taking the path from the node you wish to start from. For example, using the starting path `1/2/5/1/2`, the last digit can be recursively removed to move up through the parents. The first pass would start with the path `1/2/5/1/2`, which has the parent with the path `1/2/5/1`, whose parent is `1/2/5`, followed by `1/2` up to the root `1`. A PL/SQL procedure could be written to handle this kind of query and called in a function. Alternatively, to make the interface more responsive, the parent path for each node could be calculated by this procedure and stored in a table.

8.4 Further Work

- Delivering TCl-Db in RDF
  As stated above, it is our proposal to maintain the assertion data of TCl-Db in RDF format. This satisfies two objectives, first, delivering TCl-Db data in RDF format via RSS feeds will enable the integrated data to be shared with other resources on the web. Second

once the data sources used by TCl-Db move towards delivering data and updates via subscribed RSS feeds, this provides a very convenient mechanism of automated updates to the data that can be propagated into the database.

- Data Update
  The classification data in TCl-Db is not amenable to automatic updates, since these data need to be converted into nested sets and materialised paths before they can be loaded. Experience of manual data updates so far has enabled us to recognise where manual intervention is most often required in these updates. So far, misplaced synonyms in the classification and homonyms have caused problems. It is possible to now to make provisions for these scenarios and deal with them within an automated script.

- New Data Sources
  As stated in Chapter 3, adding new data sources to TCl-Db is very simple. Data sources are usually replicated into a separate silo and PL/SQL procedures copy the data into the TCl-Db schema. New data sources can be added within hours as need arises.

- Data Model Improvements
  Improvements to the data model will be made to better handle they way homonyms and synonyms are dealt with. These improvements will also have a positive impact on the data updates.

- Web Interface Improvements
  Additional queries will be added to the web interface and SOAP service. An ancestor query has been identified as a requirement and further additions will be made as user requirements dictate.

8.5 Other Possible Work Directions

One could imagine this research extended in a number of dimensions. The first of those is visualisation. The Treebolic viewer used in the work of E. Grant (see Chapter 2 Figure 2.3) was a good solution, but since this work was carried out, new visualisations have become available, developed mainly by the University of Maryland (http://www.cs.umd.edu/hcil/biodiversity/). One could also investigate the usability of such tree comparisons and how well they support a scientist in understanding the data and its complexities.

One could also work on the algorithmic efficiency of querying, as with the advent of even larger classifications and tree databases, more efficient data access may be required. Alternative tree representations and additional indexes could help in this work. One would typically carry out performance measurement to decide between alternative data and index layouts.

Another angle on the issues of querying would be furnished by the investigation of the changes in classification, as done in the work of (Pullan *et al.*, 2000). This will be relevant as more classifications become available and are subject to minor and major adjustments, due to our improving knowledge of phylogeny.

8.6 Conclusion

This thesis addressed data integration and query problems observed in taxonomy and systematics. Based on an analysis of query logs, we showed that the majority of queries submitted to the main phylogeny database, TreeBASE, or submitted on the web by naive users do not find the information which the users require. Based on this material, we derived a number of user requirements, and then we produced a solution which fulfils those requirements. The solution presented here consisted of a supporting database warehouse which performs query expansion with synonyms, vernaculars and hierarchically structured classification terms. This solution was evaluated and shown to be far superior to the standalone version of TreeBASE. Future work extending this thesis would consist in adding new data sources, extending the semantic power of this database warehouse, and provision and testing of improved user interfaces for tree visualisation and traversal.

This closes the thesis with the conclusion that the newly implemented database warehouse satisfies the needs of taxonomic research to a far greater extent than other existing solution and proves the research hypothesis presented at the start of the thesis.

Appendix A

SQL Queries - A

A.1 Database Utility Queries

Hierarchical Queries

A1. Count nodes contained within this genus *Crocodylus* (name_id=13232589)in the ITIS (tree_id 1).

```
SELECT count(*)
FROM node
WHERE parent_name_id = 13232589
AND tree_id = 1
```

A2. Count nodes below 13232589 (*Crocodylus*) that are have rank = species.

```
SELECT count(*), b.rank
FROM node a, assertion b
WHERE a.assertion_id = b.assertion_id
AND a.parent_name_id = 13232589
AND a.tree_id = 1
AND b.source_id = 116
GROUP BY rank HAVING count(*) > 0
```

A3. Traversing the tree from the node 13285208 (Crocodilia) using CONNECT BY:

```
SELECT node_id
FROM node
WHERE tree_id = 1
START WITH (name_id = 13285208 and tree_id = 1)
CONNECT BY PRIOR name_id = parent_name_id
```

A4. Display the path of a node up to the root, by name_id:

```
SELECT LPAD(' ', 2*level-1)| | SYS_CONNECT_BY_PATH(name_id, '/') "path"
FROM node
WHERE tree_id = 1
START WITH (name_id = 13285208 and tree_id = 1)
CONNECT BY PRIOR parent_name_id = name_id
```

A5. Display the path of a node up to the root, by name_text:

```
SELECT LPAD(' ', 2*level-1)| | SYS_CONNECT_BY_PATH(b.name_text, '/') "Path"
FROM node a, name b
WHERE a.name_id = b.name_id
AND tree_id = 1
START WITH (a.name_id = 13285208 and a.tree_id = 1)
CONNECT BY PRIOR a.parent_name_id = b.name_id
```

A6. Count species contained within the genus *Crocodylus* (name_id = 13232589) in ITIS (tree_id 1):

```
SELECT count(*)
FROM node
WHERE left_id between
(SELECT left_id FROM node WHERE name_id = 13232589 AND tree_id = 1)
AND
(SELECT right_id FROM node WHERE name_id = 13232589 AND tree_id = 1)
AND tree_id = 1
```

A7. Select the path for a node and then count how many nodes fall within that path:

```
SELECT path FROM node
WHERE tree_id = 1
AND name_id = 13232589
```

```
SELECT count(*)
FROM node
WHERE tree_id = 1
AND path like
'/1/30/3/4/4/1/1%'
```

Data Analysis Queries

A8. This query gives 48355 names common to NCBI and ITIS.
To indicate how many are species the query can be extended to
include the clause where rank='species'. (See also Figure 5.1)

```
SELECT count(*)
FROM assertion
WHERE a.source_id = 116
AND name_id in
(SELECT name_id FROM assertion WHERE source_id = 117)
```

A9. This query builds a materialized view of all known NCBI homonyms
using the NCBI schema data.

```
CREATE MATERIALIZED VIEW ncbi_homonyms AS
SELECT b.name_id, b.name_text, a.rank, a.kingdom
FROM assertion a, name b
WHERE a.name_id = b.name_id
AND b.name_usage = 'valid'
AND a.source_id = 117
AND a.dbsource_id in
(SELECT tax_id FROM ncbi.ncbi_names WHERE unique_name IS NOT NULL
AND name_class = 'scientific_name')
```

A10. The query used to build the materialized view itis_homonyms_mv
and ncbi_homonyms_mv using TCI-Db node data.

```
CREATE MATERIALIZED VIEW itis_homonyms_mv AS
SELECT get_name_text(a.name_id), get_name_text(a.parent_name_id),
get_name_text(b.parent_name_id)
FROM node a, node b
WHERE a.name_id = b.name_id
AND a.node_id != b.node_id
AND a.tree_id = 1
AND b.tree_id = 1
AND a.parent_name_id != b.parent_name_id
AND a.name_id NOT IN
(SELECT name_id FROM assertion WHERE source_id = 116 AND rank = 'Variety')
```

```
CREATE MATERIALIZED VIEW ncbi_homonyms_mv AS
SELECT get_name_text(a.name_id), get_name_text(a.parent_name_id),
get_name_text(b.parent_name_id) FROM node a, node b
WHERE a.name_id = b.name_id
AND a.node_id != b.node_id
AND a.tree_id = 2
AND b.tree_id = 2
AND a.parent_name_id != b.parent_name_id
and a.name_id !=13351800
```

A11. This query identifies how many of the synonym names in the
TCI-Db have more than one valid name associated with it.

```
SELECT count(*) FROM synonym_name a, assertion b, assertion c
WHERE b.source_id = 117
AND c.source_id = 116
AND a.name_id = b.name_id
AND a.name_id = c.name_id
```

A12. Query to identify number of unique NCBI names in each rank.

```
SELECT count(*), b.rank
FROM node a, assertion b
WHERE a.assertion_id = b.assertion_id
AND a.tree_id =2
AND a.name_id not in (
SELECT name_id FROM node WHERE tree_id= 1)
GROUP BY b.rank HAVING count(*) >1
```

```
SELECT count(*), b.rank
FROM node a, assertion b
WHERE a.assertion_id = b.assertion_id
AND a.tree_id =2
AND b.rank ='Species'
AND a.name_id not in (
SELECT name_id FROM node WHERE tree_id= 1)
GROUP BY b.rank HAVING count(*)>1
```

A13. This query identifies valid species names in the NCBI kingdom Bacteria that are not binomial.

```
SELECT count(*)
FROM name
WHERE name_id IN
(SELECT name_id FROM assertion
WHERE source_id = 117 AND kingdom = 'Bacteria' AND rank='Species')
AND name_text LIKE '% % %'
AND name_status = 'valid'
```

A14. This query uses the table name_search to find all linked names as in Figure 3.3.

```
SELECT name, valid_name
FROM name_search
WHERE name = 'Diomedea albatrus'
OR valid_name = 'Diomedea albatrus';
```

Classification comparison queries

A15. This query returns the number of names that are common to both the NCBI (tree_id 2) and ITIS (tree_id 1) classification.

```
SELECT count(*)
FROM node a, node b
WHERE a.name_id = b.name_id
AND a.tree_id = 2
AND b.tree_id = 1
```

A16. Similar to 1 above but returns the number of nodes that have different parents in the classification.

```
SELECT count(*)
FROM node a, node b
WHERE a.name_id = b.name_id
AND a.tree_id = 2
AND b.tree_id = 1
AND a.parent_name_id != b.parent_name_id
```

A17. Similar to A16 above but using the hierarchical data from the node Crocodylidae.

```
SELECT get_name_text(a.name_id) AS child,
get_name_text(a.parent_name_id) as parent_ncbi,
get_name_text(b.parent_name_id) as parent_itis
FROM
(SELECT name_id, parent_name_id
FROM node WHERE tree_id = 2
START WITH (name_id = 13232588 and tree_id = 2)
CONNECT BY PRIOR name_id = parent_name_id) a ,
(SELECT name_id, parent_name_id
FROM node WHERE tree_id = 1
START WITH (name_id = 13232588 and tree_id =1)
CONNECT BY PRIOR name_id = parent_name_id) b
WHERE a.name_id = b.name_id
AND a.parent_name_id != b.parent_name_id
```

A18. The functions used in this query, returns the full path string for a particular name_id. The functions themselves use the SYS_CONNECT_BY_PATH as in the example A4 above. The use of the functions greatly simplifies this query.

```
SELECT get_ncbi_path_string(name_id), get_itis_path_string(name_id)
FROM name
WHERE name_id = 13250043
```

Appendix B

SQL Queries - B

B.1 Taxonomic Data extraction, reconciliation and validation - SQL Queries

B1.

```
SELECT count(*)
FROM assertion
WHERE source_id = 248
AND name_id IN
(
SELECT name_id FROM assertion WHERE source_id = 247
);
```

B2.

```
SELECT get_name_text(name_id) from synonym_name
WHERE name_id in
(
SELECT name_id FROM assertion WHERE name_id IN
( SELECT name_id FROM node WHERE source_id = 117
AND left_id BETWEEN 419620 AND 432391)
AND name_id NOT IN
( SELECT name_id FROM node WHERE tree_id = 1
AND left_id BETWEEN 346067 AND 374256 )
AND source_id = 116
);
```

B3.

```
SELECT distinct(get_name_text(b.name_id)) as genus,
get_name_text(b.parent_name_id) as ncbi,
get_name_text(a.parent_name_id) as itis
FROM node a, node b
WHERE a.tree_id =1
AND b.tree_id = 2
AND a.name_id = b.name_id
AND a.parent_name_id != b.parent_name_id
AND b.name_id IN
(
SELECT name_id FROM assertion
WHERE source_id = 117 AND rank = 'Genus' AND name_id IN
(SELECT name_id FROM node WHERE tree_id = 2
AND left_id BETWEEN 419620 and 432391)
)
AND a.name_id IN
(
SELECT name_id FROM assertion
WHERE source_id = 116 AND rank = 'Genus' AND name_id IN
(SELECT name_id FROM node
WHERE tree_id = 1 AND left_id BETWEEN 346067 AND 374256)
);
```

B4.

```
SELECT distinct(get_name_text(b.name_id)) as genus,
get_name_text(b.parent_name_id) as family,
get_name_text(a.parent_name_id) as itis
FROM node a, node b
WHERE a.tree_id =1
AND b.tree_id = 2
AND a.name_id = b.name_id
AND a.parent_name_id != b.parent_name_id
AND b.name_id IN
(
SELECT name_id FROM assertion
WHERE source_id = 117 AND rank = 'Genus' AND name_id IN
(SELECT name_id FROM node WHERE tree_id = 2
AND left_id BETWEEN 419620 AND 432391)
)
AND a.name_id IN
(
SELECT name_id FROM assertion
WHERE source_id = 116 AND rank = 'Genus' AND name_id IN
(SELECT name_id FROM node WHERE tree_id = 1
AND left_id BETWEEN 346067 AND 374256)
)
AND b.parent_name_id IN
(SELECT name_id FROM assertion
WHERE source_id = 117 AND rank = 'Family' AND name_id IN
(SELECT name_id FROM node WHERE tree_id = 2
AND left_id BETWEEN 419620 AND 432391)
)
AND b.parent_name_id IN
(SELECT name_id FROM synonym_name)
;
```

Appendix C

SQL Queries - C

C.1 Taxonomic requirements of TreeBASE

C1.

```
SELECT count(distinct(treeid))
FROM treetaxa WHERE taxonid IN
(SELECT a.taxonid FROM taxa a, treebase_queries_distinct b
WHERE lower(a.taxonname) = lower(b.query))

SELECT count(distinct(matrixid))
FROM matrixtaxa WHERE taxonid IN
(SELECT a.taxonid FROM taxa a, treebase_queries_distinct b
WHERE lower(a.taxonname) = lower(b.query))

CREATE MATERIALIZED VIEW queries_resultcount AS
SELECT a.id, b.query, count(distinct(b.treeid))
FROM treebase_queries_distinct a, treetaxa b, taxa c
WHERE b.taxonid = c.taxonid
AND lower(a.query) = lower(c.taxonname)
GROUP BY a.id, a.query, b.treeid
HAVING count(b.treeid) >0
```

C2.

```
SELECT count(distinct(a.name_id)), b.name_status
FROM queries_matched_2 a, whouse.name b
WHERE a.name_id = b.name_id
GROUP BY b.name_status
HAVING count(a.name_id) >0
```

C3.

```
SELECT count(distinct(a.name_id)), b.rank
FROM queries_matched_2 a, whouse.assertion b
WHERE a.name_id = b.name_id
GROUP BY rank
HAVING count(a.name_id) >=1
```

C4.

```
SELECT count(distinct(a.name_id)), get_source_name(source_id)
FROM whouse.assertion
WHERE name_id IN
(select name_id from treebase_queries_matched_2)
GROUP BY source_id
HAVING count(*)>0

SELECT count(distinct(name_id)) as cnt,
get_source_name(source_id) as source
FROM whouse.assertion
WHERE name_id IN
( SELECT name_id FROM treebase06.queries_matched_2
WHERE lower(query) IN
(SELECT lower(a.taxonname) FROM treebase06.taxa a, treebase06.treetaxa b
WHERE a.taxonid=b.taxonid)
) GROUP BY source_id
HAVING count(*)>0
```

C5.

```
SELECT a.query, a.q_count,
get_name_text(b.valid_name_id) name,
count(distinct(c.treeid))
FROM treebase06.treebase_queries_distinct a,
whouse.vernacular b,
treebase06.treetaxa c,
treebase06.taxa d
WHERE lower(a.query) = lower(get_name_text(b.name_id))
AND c.taxonid = d.taxonid
AND lower(d.taxonname) = lower(get_name_text(b.valid_name_id))
GROUP BY a.query, a.q_count, b.valid_name_id
HAVING count(c.treeid)>0
ORDER BY a.q_count DESC
```

C6.

```
SELECT count(distinct(name_id))
FROM node
WHERE parent_name_id =
( SELECT name_id FROM name WHERE name_text = 'Aspergillus')
```

C7.

```
SELECT count(distinct(b.treeid))
FROM treebase06.taxa a, treebase06.treetaxa b
WHERE a.taxonid= b.taxonid
AND LOWER(a.taxonname) IN
(SELECT LOWER(get_name_text(name_id)) FROM node WHERE parent_name_id =
(SELECT name_id FROM name WHERE name_text = 'Aspergillus')
GORUP BY name_id)
```

C8.

```
SELECT count(distinct(a.treeid))
FROM treebase06.treetaxa a, treebase06.taxa b
WHERE lower(taxonname) IN
(SELECT LOWER(get_name_text(name_id))
FROM whouse.node WHERE tree_id = 47 AND left_id
BETWEEN
(SELECT left_id FROM whouse.node
where tree_id = 47 AND name_id=13126098)
and
(SELECT right_id FROM whouse.node
WHERE tree_id = 47 AND name_id=13126098) )
AND a.taxonid=b.taxonid
```

Appendix D

TCl-Db in RDF

Support for RDF is provided through the Oracle Database 10g RDF Data Model (Alexander *et al.*, 2004; Murray, 2005). There are several RDF data stores with, 3store (Harris & Gibbins, 2003), Sesame (Broekstra *et al.*, 2002) and Jena2 (Wilkinson *et al.*, 2003) being the most popular (and robust). Apart from the fact that TCl-Db was already implemented within an Oracle database, the advantage of using Oracle is that queries are SQL based therefore, queries already performed in previous chapters could be easily translated. The Oracle RDF implementation is delivered within Oracle spatial which consists of a network data model (data are modelled in nodes and links). RDF triples are stored as a logical graph within spatial. The subject and objects are mapped to nodes and predicates are mapped to links, the start node of a link being the subject and the end node being the object. The way data are stored there are no repeated values, an object or subject are stored only once. This optimised storage structure maintains fidelity and means it can scale to very large datasets. RDF fits into the network model within Oracle spatial and the features that Oracle has already provided within this product for storage and retrieval of network data made this the system of choice for testing the use of RDF within TCl-Db.

The basic steps to using RDF in Oracle require first creating an RDF network, then creating the table to store the references to the RDF triples and finally creating a model that references the table in which the triples are referenced. These steps are outlined below.

1. Create tables to store the references to the RDF data

```
CREATE TABLE assertions_rdf (id NUMBER, triple SDO_RDF_TRIPLE_S);
CREATE TABLE names_rdf (id NUMBER, triple SDO_RDF_TRIPLE_S);
```

2. Create the RDF Models

```
EXECUTE SDO_RDF.CREATE_RDF_MODEL('assertions', 'assertions_rdf', 'triple');
EXECUTE SDO_RDF.CREATE_RDF_MODEL('names', 'names_rdf', 'triple');
```

3. Create Oracle database indexes on conditions that will be specified in the WHERE clause of SELECT statements, to provide better performance for such queries.

```
CREATE INDEX asertions_sub_idx ON assertions_rdf (triple.GET_SUBJECT());
CREATE INDEX asertions_prop_idx ON assertions_rdf (triple.GET_PROPERTY());
CREATE INDEX asertions_obj_idx ON assertions_rdf (TO_CHAR(triple.GET_OBJECT()));
CREATE INDEX asertions_tri_idx ON assertions_rdf (triple.rdf_t_id);
CREATE INDEX names_sub_idx ON names_rdf (triple.GET_SUBJECT());
CREATE INDEX names_prop_idx ON names_rdf (triple.GET_PROPERTY());
CREATE INDEX names_obj_idx ON names_rdf (TO_CHAR(triple.GET_OBJECT()));
CREATE INDEX names_tri_idx ON names_rdf (triple.rdf_t_id);
```

TCl-Db in RDF

The default method used for describing RDF data models is the RDF graph, these are simple directed graphs with labelled nodes and edges. While RDF graph is used to model the data the format for delivering the data in an RDF graph is through serialisation using RDF/XML (Beckett *et al.*, 2003). The TCl data mapped into RDF is shown in Figure D.1. Relational tables are easily serialised into RDF/XML using SQLX. The SQLX queries for the tables ASSERTION,

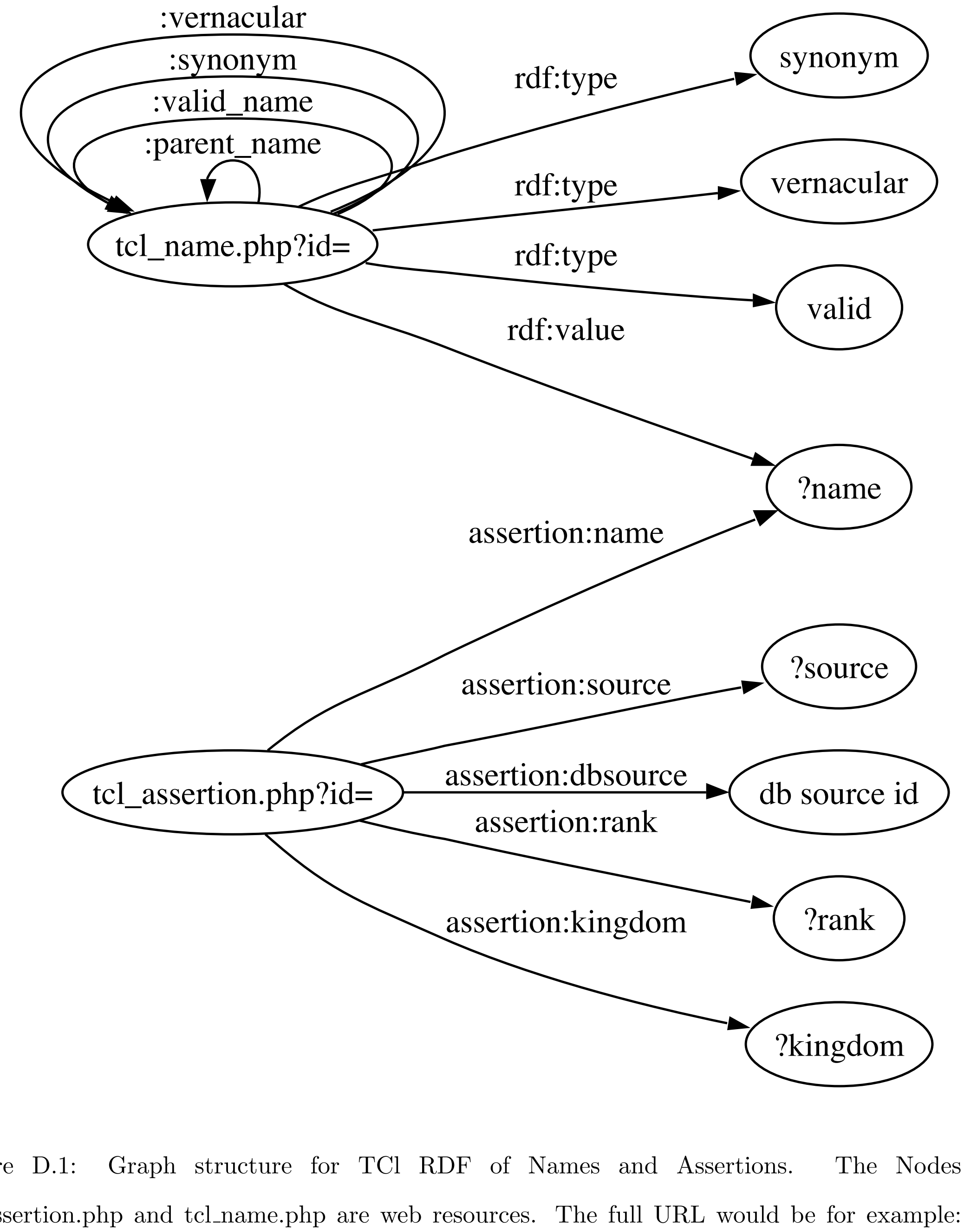


Figure D.1: Graph structure for TCl RDF of Names and Assertions. The Nodes tcl_assertion.php and tcl_name.php are web resources. The full URL would be for example: http://spira.zoology.gla.ac.uk/tcl_name.php?id=13232598

NAME and NODE tables are given below.

- ASSERTION SQLX

```
select XMLELEMENT("rdf:description",
XMLATTRIBUTES(a.assertion_id as
         "rdf:about=http://spira.zoology.gla.ac.uk/tcl_assertion.php?id"),
XMLELEMENT("assertion:source", get_source_name(source_id)),
XMLELEMENT("assertion:dbsourceid", dbsource_id),
XMLELEMENT("assertion:rank", rank),
XMLELEMENT("assertion:kingdom", kingdom),
XMLELEMENT("assertion:name",
XMLATTRIBUTES(get_name_text(name_id) as
           "rdf:resource=http://spira.zoology.gla.ac.uk/tcl_name.php?id"))
)
from assertion a
```

- NAME SQLX

```
select XMLELEMENT("rdf:description",
XMLATTRIBUTES(a.name_id as
         "rdf:about=http://spira.zoology.gla.ac.uk/tcl_name.php?id"),
XMLELEMENT("name:text", a.name_text),
XMLELEMENT("name:status", a.name_status),
XMLELEMENT("name:synonym", get_name_text(b.name_id)),
XMLELEMENT("name:vernacular", get_name_text(c.name_id)),
XMLELEMENT("name:parent",
XMLATTRIBUTES(d.parent_name_id as
           "rdf:resource=http://spira.zoology.gla.ac.uk/tcl_name.php?id"))
)
from name a, synonym_name b, vernacular c, node d
where a.name_id = b.valid_name_id
and a.name_id = c.valid_name_id
and a.name_id = d.name_id
```

These queries return three XML files, when edited to include the appropriate headers, these would then be parsed using XSLT (using for example the XALAN processor) into Notation 3 format (N3) (Berners-Lee, 2006). The XSLT script is given in Appendix A. The Oracle RDF loader uses Java to load data in N3 format. Similarly, XSLT can be used to build SQL insert statements that can be directly executed from sqlplus utility, however the Java loader performs much better than individual insert statements. The command line:

```
java -classpath .:$ORACLE_HOME/jdbc/lib/ojdbc14.jar:./sdordfclient.jar
         TestNTriple2NDM  name.nt name_rdf names 12
```

for example, would load the NAME file in N3 format into the table NAMES_RDF, these data would be associated with the model NAMES which has a model id of 12.

TreeBASE in RDF

The RDF model for TreeBASE is given in Figure D.2. Using the TreeBASE schema that was replicated into the local Oracle database, a similar SQLX query would serialise the data into RDF/XML. The queries for the TREETAXA and the MATRIXTAXA tables are given below. Again, with the addition of the appropriate headers, these files would be parsed with XSLT (Appendix B) into N3 format and loaded into Oracle as shown above.

- TREEBASE.MATRIXTAXA SQLX

```
select XMLELEMENT("rdf:description",
XMLATTRIBUTES(b.matrixid as
      rdf:about="http://spira.zoology.gla.ac.uk/treebase_matrix.php?id),
XMLELEMENT("matrixtaxa:taxonid",
XMLATTRIBUTES(b.taxonid as
      rdf:resource="http://spira.zoology.gla.ac.uk/treebase_taxon.php?id)),
XMLELEMENT("taxa:name", c.taxonname)
)
from matrixtaxa b, taxa c
where b.taxonid = c.taxonid
```

- TREEBASE.TREETAXA SQLX

```
select XMLELEMENT("rdf:description",
XMLATTRIBUTES(b.treeid as
     rdf:about="http://spira.zoology.gla.ac.uk/treebase_matrix.php?id),
XMLELEMENT("treetaxa:taxonid",
XMLATTRIBUTES(b.taxonid as
     rdf:resource="http://spira.zoology.gla.ac.uk/treebase_taxon.php?id)),
XMLELEMENT("taxa:name", c.taxonname)
)
from treetaxa b, taxa c
where b.taxonid = c.taxonid
```

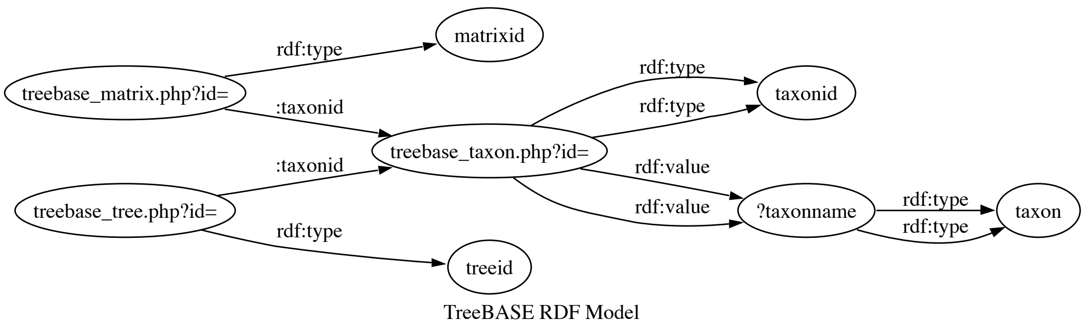


Figure D.2: Graph structure for TreeBASE.

Querying TCl-RDF

As described in previous chapters, the content and design of TreeBASE does not enable effective data retrieval using taxon names. While TreeBASE does have an element of taxonomy through the tables TAXON, TREETAXA and MATRIXTAXA, these data do not include the full hierarchy and linked alternative names, thus searches using taxon names may not return all the data a user would expect. This thesis outlines the use of a data warehouse that can be integrated into TreeBASE to enable the types of taxon searches that were described in Chapter 5. Semantic technologies, RDF, RDFS etc., give a new alternative to traditional integration and mapping of data. As described above data delivered in RDF forms a graph, two datasets brought together in this format can be easily queried together, the architecture is depicted in Figure D.3. While RDF provides a means of integration over data, the purpose of integrating data is to allow the data to be queried together. Several query languages have been proposed for querying RDF data, SPARQL query language for RDF (Prudhommeaux & Seaborne, 2004) and RDQL, RDF Data Query Language (Seaborne, 2004) are implementations that have been submitted to the W3C. Oracle has implemented SPARQL like graph patterns for querying RDF within Oracle Spatial.

The use of semantic integration is exemplified here with the TCl RDF data model and TreeBASE RDF model for TREETAXA and MATRIXTAXA tables. The query possibilities through these RDF data are given with some examples below using the model given in Figure D.4. The last query is an example of the use of data in both the network model and relational model.

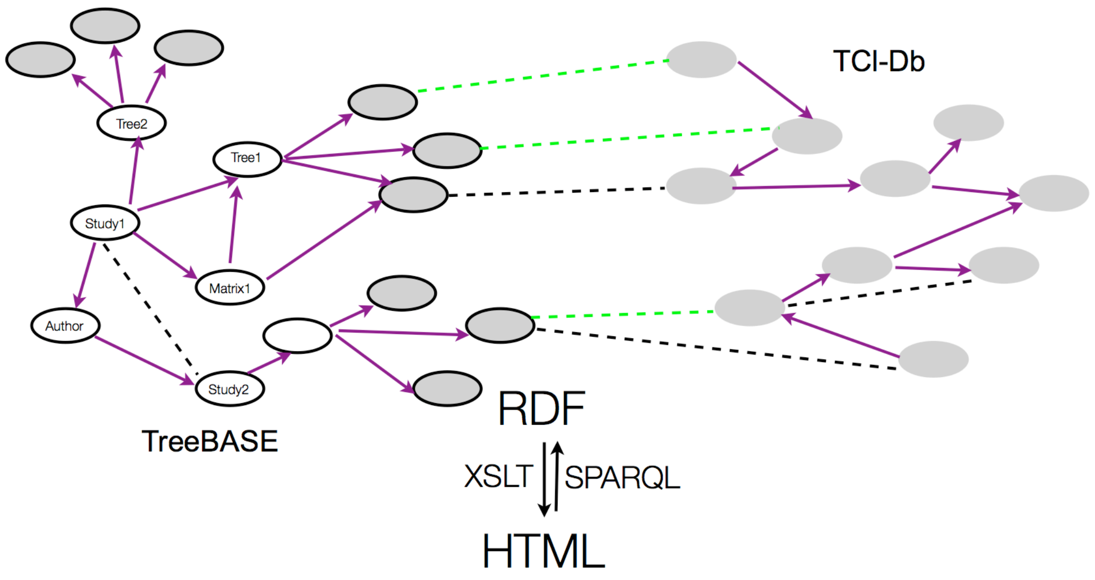


Figure D.3: The diagram above represents how two RDF graphs can be brought together and integrated through inference rules. The dashed lines in green depict the mapping of identical nodes in the two trees and the black dashed line depicts how new triples can be inferred from rules and existing triples. When the datasets are brought together in RDF format, they can be queried together using SPARQL embedded within SQL. The result set of such a query can be easily parsed via XSLT into HTML for inclusion within a web interface.

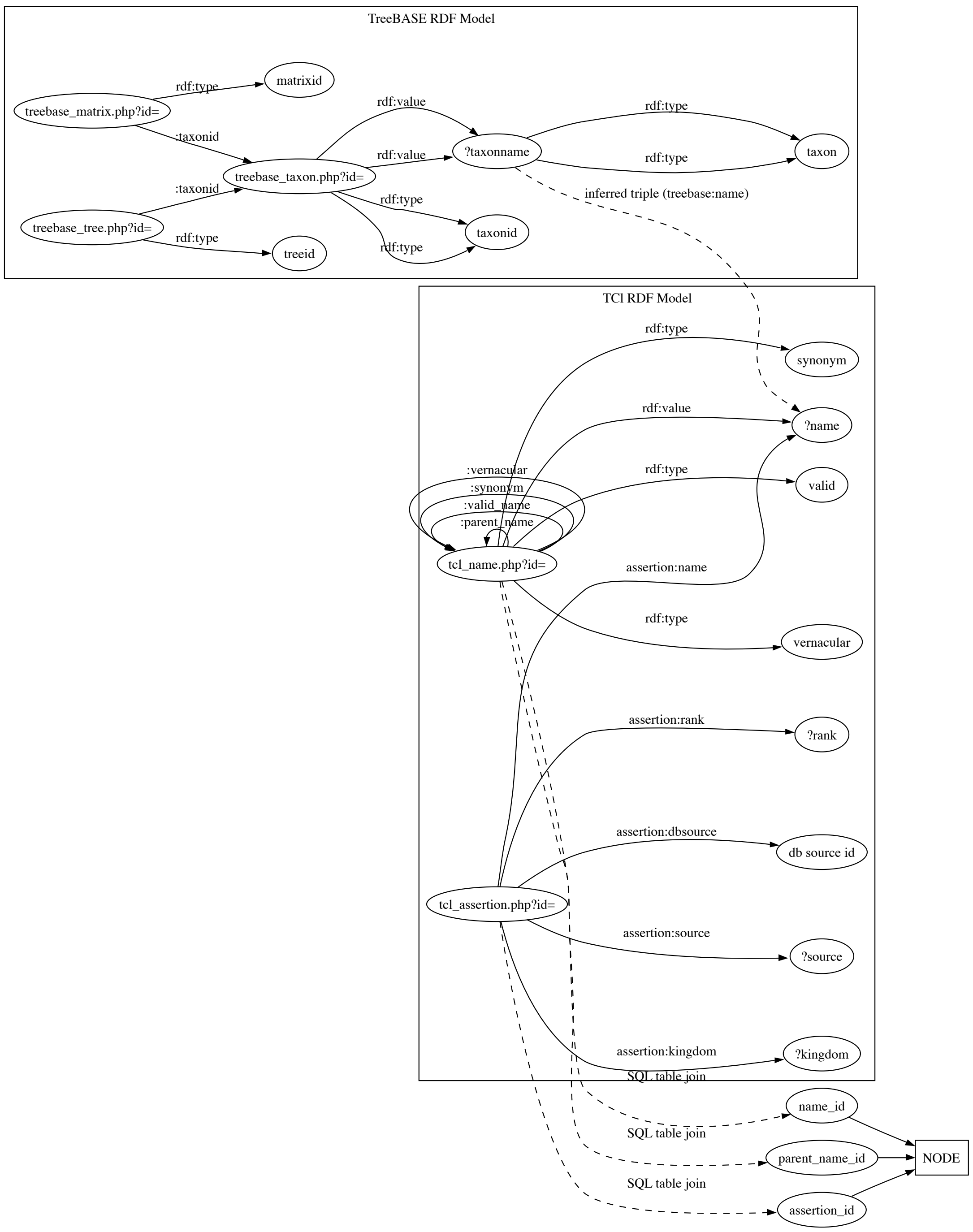


Figure D.4: RDF graph for TCl and TreeBASE RDF model. The dashed line connecting the nodes taxonname and name_text represents the inferred triple, using this triple the two data sets can be queried together. i.e treebase data can be queried using taxa names. In Oracle data in the network data model and the relational data model can be queried together through SQL. Using the data in the relational NODE table traditional hierarchical queries can be combined with the RDF queries.

Data Retrieval Queries

- selects all valid names for synonyms

```
select nameid, name
from TABLE(SDO_RDF_MATCH(
   '(?nameid :synonym ?x)
   (?x rdf:value ?name)',
SDO_RDF_MODELS('names'),
null,
SDO_RDF_ALIASES(SDO_RDF_Alias('', 'http://spira.zoology.gla.ac.uk/terms/TCL/')),
null));
```

- selects all valid names for the vernacular “hazelnut”

```
select  name
from TABLE(SDO_RDF_MATCH(
   '(?nameid :vernacular ?x)
   (?x rdf:value "hazelnut")
   (?nameid rdf:value ?name)',
SDO_RDF_MODELS('names'),
null,
SDO_RDF_ALIASES(SDO_RDF_Alias('', 'http://spira.zoology.gla.ac.uk/terms/TCL/')),
null));
```

- select TreeBASE treeids

```
select treeid, taxonid, name
from TABLE(SDO_RDF_MATCH(
   '(?treeid rdf:type :treeid)
   (?treeid :taxonid ?taxonid)
   (?taxonid rdf:value ?name)
   (?name rdf:type :taxon)',
SDO_RDF_MODELS('treebase'),
null,
SDO_RDF_ALIASES(SDO_RDF_Alias('', 'http://spira.zoology.gla.ac.uk/terms/TCL/')),
null));
```

- TreeBase Inference

```
EXECUTE SDO_RDF_INFERENCE.CREATE_RULEBASE('taxon_rb');
INSERT INTO mdsys.rdfr_taxon_rb VALUES(
  'parent_rule',
  '(?treebasename rdf:type :taxon)
  (?nameid rdf:type ?valid)
  (?nameid rdf:value ?whousename)',
NULL,
'(?treebasename :links ?whousename)',
SDO_RDF_Aliases(SDO_RDF_Alias('','http://spira.zoology.gla.ac/terms/TCL/links')));
```

- TreeBase query using inference rule

```
select a.treeid, a.nameid, b.parent_name_id
from TABLE(SDO_RDF_MATCH(
  '(?treeid rdf:type :treeid)
  (?treeid :taxonid ?taxonid)
  (?taxonid rdf:type :taxonid)
  (?taxonid rdf:value ?taxon)
  (?taxon :links ?name)
  (?nameid rdf:value ?name)
  (?name rdf:value "Candida")',
SDO_RDF_MODELS('names'),
SDO_RDF_RULEBASES('RDFS','taxon_rb'),
SDO_RDF_ALIASES(SDO_RDF_Alias('', 'http://spira.zoology.gla.ac.uk/terms/TCL/')),
null)) a, whouse.node b
where a.nameid=b.name_id
```

- TreeBase TreeIDs from a higher taxa name query using spatial and relational tables

```
select treeid
from TABLE(SDO_RDF_MATCH(
  '(?treeid rdf:type :treeid)
  (?treeid :taxonid ?taxonid)
  (?taxonid rdf:type :taxonid)
  (?taxonid rdf:value ?taxon)
  (?taxon :links ?name)
  (?nameid rdf:value ?name)
  (?name rdf:value "Candida")',
SDO_RDF_MODELS('names'),
SDO_RDF_RULEBASES('RDFS','taxon_rb'),
SDO_RDF_ALIASES(SDO_RDF_Alias('', 'http://spira.zoology.gla.ac.uk/terms/TCL/')),
null));
```

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