Overcoming the limitations of PDB format

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ABSTRACT

The Protein Data Bank is a repository for the 3-D structural data of large biological molecules, such as proteins and nucleic acid. The PDB is a key resource in the areas of structural biology, structural genomics. Most major scientific journals, and some funding agencies, such as the NIH in the USA, now require scientists to submit their structure data to the PDB. If the contents of the PDB are thought of as primary data, there are hundreds of derived databases that categorize the data differently. For example, both SCOP and CATH categorize structure according to type of structure and assumed evolutionary relations; GO categorize structures based on genes. In this paper, we will describe how to overcome the limitations of PDB format.

Keywords: PDB, XML, XCML.

INTRODUCTION:

Protein Data Bank

The Protein Data Bank was established at Brookhaven National Laboratories in 1971 as an archive for biological macromolecular crystal structures. In the beginning the archive held seven structures, and with each year a handful more were deposited. In the 1980’s the number of deposited structures began to increase dramatically. This was due to the improved technology for all aspects of the crystallographic process, the addition of structures determined by the nuclear magnetic resonance (NMR) methods, and changes in the community views about data sharing.

PDB Data Curation

It is well known that the human genome project has resulted in rapidly growing databases in bioinformatics. And bioinformatics provide some opportunities to develop novel data analysis method, but there are still some challenges including protein structure prediction, genomic sequence analysis, etc. For example in protein structure prediction, scientists are using PDB file to apply amino acid sequence to determine the secondary and tertiary structure of proteins.

Unfortunately, PDB supports several different formats, thus it suffers from inconsistencies in how the data formats are constructed over time. PDB format is old, ambiguous and inadequate, but it is still the most widely used format since all relevant software can read it. Although some users claim they do not mind the errors of PDB file, which may result in the partial or wrong information to affect the accuracy of derived and propagated data. Thus it is very necessary to develop a system to curate data in PDB file, to provide easy understanding and better services for protein scientists and computer scientists.

There are two architectures for PDB data curation : one simply uses checking filter and curation engine to curate data. The other one uses the first one by adding XCML curation part to further curate data, which can deeply clean the PDB data by using more constraints. These two tools can be used not only for cleaning existing PDB files and also for creating new PDB files.

Figure1. PDB Data curation system architecture

The above picture shows the architecture for PDB data curation system. From user interface, checking filter gets PDB file, which checks the error and reports them to curation engine, and then curated data by curation engine are sent to database storage. The users can get better PDB file from our database after this process.

Most errors are fixed in original PDB file after it is through this PDB data curation system. But however, still some issues related to interoperability with the latest technology are still left, which may again can create errors.

Architecture of PDB Data Curation System with XCML

The Extensible Markup language (XML) is self describing, and is standardized by the World Wide Web Consortium (W3C). It is human and machine readable, flexible, extensible and has already became the standard format for exchanging the information through the network. It usually uses the XML schema or document type definition (DTD) to define syntax and data types. But it can not verify semantic constraints, avoid erroneous data and is domain dependent. Therefore we will not get any better data if we just convert PDB file into XML format. In order to avoid disadvantages of XML and make use of XML’s metrics to get better data, we apply an XML constraint language, extensible constraint markup language (XCMML), which is more powerful.

The following architecture shows how to improve our PDB data curation system by using XCMML. Firstly PDB file is submitted to PDB data curation system, after curation, PDB file can be converted into XCMML format by converter XML, which uses some constraints to further curate. PDB-XCMML can be in protein-OODB format after it is handled by converter PDB and converter OODB. At this moment users can get better data that are in domain specific object-oriented format.
**Figure 2.** Below diagram shows the architecture of PDB Data curation system.

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**Problem with Protein data bank**

With the passage of time, numerous research initiatives are coming to a level of maturity, in which the biological data size have become exponentially big as well as leading to data inconsistency problems like Formatting, Ambiguous data, Data identification, Data Errors, Redundant data, interoperability of the legacy biological data with the current technologies. Therefore there is an urgent need to overcome these issues. So we need to develop a framework which can bridge the connectivity of these old legacy database technologies with new contemporary technologies like DB4o.

Since, the PDB file needs a special text processing functions for its extraction of information for usage in bioinformatics applications, there is a need to reduce the need for more text processing and have a simple framework in which the queries are simple to process and data can be represented as objects for its maximum maintainability.

The text processing required to process the PDB file takes extra efforts and resources. For example in certain area the coordinate values get merged with each other and it is very difficult to process and get separate coordinate values based on white space and delimiters. So we need to overcome these typical issues and move ahead with contemporary technology integration.

Also it is not clear whether the residue name is 2, 3 or 5 digit or alphabet, they also get merge. It is also difficult to process and get separate coordinate values as it gets merged with the next column value.

**DB4o**

DB4o is an embeddable open source object database for JAVA and .NET developers. DB4o is written in JAVA and .NET and provide the respective API’s. DB4o can run on any operating system that supports JAVA and .NET.

DB4o represents an object-oriented data base model. One of its main goal is to provide an easy and native interface to persistence for object-oriented languages. Development with DB4o database does not require a separate data model creation; the applications class model defines the structure of the data in DB4o database. DB4o attempts to avoid the object/relational impedance mismatch by elimination the relational layer from a software project.

**Features of DB4o database**

**One-line-of-code database**

DB4o contains a function to store any object with a single command:

```
ObjectContainer.Store(New SomeClass());
```

**Embeddable**

DB4o is designed to be embedded in clients or other software components completely invisible to end-user. Thus DB4o needs no separate installation mechanism, but comes as just one easily deployable library with a very low footprint of ~670 kb in .NET version and around 1MB in java version.

**Client-Server mode**

Client/Server version allows DB4o to communicate between client and server-side applications. DB4o uses TCP/IP for client-server communication and allows configuring port number. Communication is implemented through messaging.

**Dynamic Schema Evolution**
DB4o supports automatic object schema evolution for the basic class model changes. More complex class model modifications, like field name change, field type change, hierarchy move are not automated out-of-the-box, but can be automated by writing small utility update program.

This feature can be viewed as an advantage over relational model, where any change in schema results in mostly manual code review and upgrade to match the schema changes. In most cases the code upgrade can not be automated as the actual query language is string based (SQL) and is not recognized by IDE auto completion and code generation tools like intellisense.

Native Queries
Rather than using string-based API’s (such as SQL, OQL), programming language itself to access the database and thus avoid a constant, productively-reducing context switch between programming language and data access API.

LINQ
LINQ support is fully integrated in DB4o for .NET version 3.5. LINQ allows creating object-oriented queries of any complexity with the benefit of any complexity with the benefit of compile time checking, IDE intellisence integration and automated refactoring.

Due to integration with some open-source libraries DB4o allows optimized LINQ queries on compact framework.

LINQ can be used both against relational and object data storage, thus providing a bridge between them, which can be valued for projects using both technologies, or for project migration between the two. It can also be used as an abstraction layer, allowing to easily switch the underlying database technology.

Portability and cross-platform deployment
DB4o was successfully tested on java FX and Silverlight.

DB4o runs out of the box on Android.

DB4o uses a custom feature called “generic reflector” to represent class information, when class defamations are not available, which allows to use it in a mixed java-.NET environment, for example java client-.NET server and vice-versa.

Documentation and Support
DB4o provides various sources of documentation: tutorial, reference documentation, API documentation, online pair casts and blogs.

Object Manager
Object Manager Enterprise (OME) is a DB4o database browsing tool. Object Manager Enterprise allows to browse classes and object in the database, connect to a database server, build queries using drag and drop, view database statistics etc.

In addition to graphic interface to DB4o database OME provides some administrative functions are:
- Indexing
- Defragmentation
- Backup

Community

Over the years the community of DB4o registered members has grown to over 60,000 members. Many important DB4o related projects, such as standalone project manager, encryption support, Mono support etc, are fully driven by community members.

DB4o provides free access to its code, documentation, forums and releases to the community members. From time to time, DB4o holds different contests allowing the community members to come up with the best suggestion for an improvement of a specific DB4o aspect, which are later on integrated into the core code.

Conclusion
From the above discussion it is clear that by converting PDB file into DB4o, all the problematic issues of PDB file such as Data identification, Data Errors, Redundant data and ambiguous data can be avoided. So better version of PDB file is obtained after this conversion.

Future Work
For future directions we suggest that one should study more biological databases, which need attention sue to scope of their research and applications.

They also need high level of text processing before they can be used and require some bridging technology which can help them to be utilized with contemporary technologies like cloud applications. Therefore for future we suggest that work should be done to develop such conversion and bridging technologies which would help other legacy data sets to be used efficiently and high usage value.

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