

# Exp-DB: Fast Development of Information Systems for Experiment Tracking

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**Abstract.** Bioinformatics research groups require information systems keeping track of experiments and their results. However, current solutions are often ad-hoc, difficult to maintain, extend, or use in different context. This paper presents Exp-DB, an infrastructure for the fast development of information systems for experiment tracking. Exp-DB provides a basic, extensible database design, modular components for accessing the data, and a web-based interface. It allows for fast implementation of an initial system even by non IT-experts which can then be extended step-by-step.

## 1 Introduction

Bioinformatics research is driven by experiments. Typically, experiments are executed in form of a workflow: related experiments are executed in a predefined order and might depend on each other. We refer to a set of such related experiments as *experiment workflow*. With the introduction of new technology, more and more experiments are automated leading to an explosion in the number of experiments and a need for computer supported analysis of conducted experiments. As a result, many research groups have started to develop web-based information systems that keep track of their experiments, e.g., [2, 5, 6]. The initial investment in building such systems can be quite high. Since these systems are seldomly built by computer scientists, the team members first have to learn the essentials of the technology. Due to fuzzy requirements, time pressure and lack of experience, the developed systems often lack modularity and extensibility, and are only usable in very specific context.

Exp-DB attempts to address these issues. It is a multi-tier infrastructure intended to help small scientific research groups to develop their own information system for experiment tracking. The development of Exp-DB was motivated by two goals. Firstly, the design, architecture, and infrastructure must be simple enough to be understood in reasonably short time by people without extensive computer skills. This is needed to have a first running system in short time. Secondly, the system must provide sufficient modularity and flexibility such that it can be extended, adjusted and optimized in many different ways (although this might require more computer science knowledge than the first step).

The architecture of Exp-DB follows a strict separation of tasks: data storage, application logic, and presentation logic are implemented in separate components. Within each of the components, different concepts are implemented

separately from each other in different modules. The architecture is based on Java Technology and uses Apache/Tomcat as its execution environment.

A research group develops its own system based on Exp-DB in the following steps. Exp-DB provides an initial, quite simple relational data model. Relying on the basic structure of the Exp-DB data model, attributes have to be added to existing tables, and new tables have to be created reflecting the particular research conducted. For instance, for each type of experiment, typically one additional table has to be added to the database plus some indication how this experiment type is related to other experiment types. For each newly created table, one small application logic program has to be generated. No further work is required to get a first running system. Web-pages are automatically generated from the entered information. The tasks to be performed require moderate knowledge in relational database design, and basics in Java programming.

There exist several databases keeping track of scientific experiments, e.g., [5, 6, 3]. General laboratory systems are e.g., [4, 7, 1, 8]. However, none of these system provides the general functionality and simplicity of our system.

## 2 Experiments and Workflows

Our system design was motivated by the existing information system of the Macromolecular Structure Group at the Biotechnology Research Center, National Research Council, Canada. This group is engaged in finding the structure of proteins mainly through x-ray crystallography. Their suite of experiments follows a typical pattern. A workflow starts with (1) selecting a set of genes or subsequences of genes as promising targets. For each selected target the further steps include (2) cloning, (3) protein production, (4) purification, (5) crystallization, (6) X-ray crystallography, and (7) structure analysis. (8) An alternative method following step (5) is NMR (nuclear magnetic resonance) spectrometry. (9) Optional quality testing occurs after the purification step (4). (10) Also, if steps (5) to (8) are unsuccessful, fragmentation splits the proteins retrieved in step (4) into smaller fragments that might be easier to crystallize. Steps (2) to (4) might be skipped if the proteins are provided by other labs.

From this description, we can introduce the following definitions. An **experiment type** describes a specific form of experiment, e.g., *Cloning*, *Purification*, etc. An **experiment** is an instance of an experiment type. An **experiment workflow** is a directed graph. Each node depicts an experiment. An edge from experiment E1 to experiment E2 indicates that E1 was performed before E2 and its output served as input for E2. Experiments are not randomly combined to experiment workflows but usually follow standard workflow patterns. That is, an experiment of type T1 might typically follow an experiment of type T2 (e.g., *Purification*  $\rightarrow$  *Crystallization*). Some patterns, however, are impossible (e.g., *Crystallization*  $\rightarrow$  *Purification*). This means, we have to restrict experiment workflows to only allow meaningful transitions between experiment types. A **workflow model** a directed graph where nodes are experiment types. An arrow from experiment type T1 to experiment type T2 indicates that the output of

an experiment of type T1 can (but need not) be input of an experiment of type T2. From there, a **legal workflow** is an experiment workflow such that for each arrow from experiment E1 of type T1 to E2 of type T2 in the workflow graph, the workflow model graph has an arrow from T1 to T2. A workflow can have one-to-many and many-to-one relationships. That is, experiment E1 of type T1 can have edges to experiments E21 and E22 both of type T2 as long as there is an arrow from T1 to T2 in the model (one purification experiment is input for many crystallization experiments). In a similar way, many experiments of the same type can be input to one further experiment (e.g. the results of many x-ray crystallography experiments can be input for a single structure analysis).

### 3 Database Design

Exp-DB distinguishes different types of information. *Access control* information is needed to restrict access to the system. *Special information* is very specific to a given research environment, e.g., information about genes and proteins. *Meta information* keeps track of the structure of the tables and their attributes. This is needed for presenting data correctly and for type checking. *Experimental information* is the backbone of the schema. The **Experiment** table contains general information about each experiment independent of the experiment type. Type dependent information is stored in separate tables, one for each type. The table **Workflow** is used to store information about conducted workflows by indicating parent and child experiments. The workflow model graph is encoded into the **Workflow Model** table. Whenever a user wants to enter a record into the **Workflow** table, the system checks in the **Workflow Model** table whether such an experiment flow is legal.

### 4 Architecture and Implementation

The system has a three-tier architecture and follows standard software development guidelines. Users (client tier) interact with the system through a standard browser. The middle tier is responsible for the presentation and business logic, and uses an Apache Tomcat web-server. The system is based on the the MVC (Model View Controller) architecture. This helps to provide a clean separation between the presentation and the processing of data. The presentation logic generates the webpages using JavaServer Pages (JSP). The JSPs represent the "View" that the users receive from the system. The application logic is implemented as a combination of Servlets and JavaBeans. The JavaBeans encapsulate the data access to the database system and represent the data in an abstract interface to JSPs and Servlets. They implement the "Model". Finally, the Servlets "control" how the user interacts with the system, and how the different components should be called. The backend tier can be any relational database system.

The system consists of several modules. Each module consists of a set of JSPs and JavaBeans that implement a specific functionality: users can enter new information (e.g., new experiments), search the database, or access specific existing

entries in the database. All requests are filtered through a controller servlet that forwards it to the corresponding module. The *non-experiment* module is responsible for entering individual entries to non experimental tables. It has a single JSP that is valid for all tables, and a JavaBean for each table. It is completely hidden from the JSP how the data is internally stored since all data access is passed through the JavaBean. The *experiment* module is more complex since the addition of an experiment requires entries into several tables and the experiment must be linked to a specific workflow. The user is guided through a sequence of web-pages to enter all relevant information. Correctness checks are performed to guarantee that only legal workflows are allowed. The *query module* provides a set of predefined queries that are typical for experimental databases. Furthermore, the user can ask more complex queries in form of SQL queries or through a query wizard. The *record module* provides the functionality to view, modify, and delete an individual existing record. For each of these methods, there exists one single JSP (independently of the table). This JSP calls the corresponding JavaBean of the table to retrieve or store the data, and then dynamically generates the webpage. Furthermore, this module provides navigation through an experiment workflow. Starting with the view of an experiment, the user can navigate to the child experiments or parent experiments.

Exp-DB only provides the basic framework and must be extended to become operational. The most typical extension will be the addition of new experiment types and the specification of the workflow model. This can be done very easily by adding new tables to the database and creating a few JavaBeans (templates are provided). Special extensions are possible due to Exp-DB's modular structure.

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