

Life Sciences Data and Application Integration with B-Fabric

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Summary

In this demo paper, we sketch B-Fabric, an all-in-one solution for management of life sciences data. B-Fabric has two major purposes. First, it is a system for the integrated management of experimental data and scientific annotations. Second, it is a system infrastructure supporting on-the fly coupling of user applications, and thus serving as extensible platform for fast-paced, cutting-edge, collaborative research.

1 Introduction

Core facilities like the Functional Genomics Center Zurich (FGCZ) typically face with the problem of efficiently supporting research. On the one hand, the usage of the facility, i.e., the access to its instruments and staff, must be coordinated. On the other hand, the huge amounts of data generated with the instruments and applications of the facility must be managed, made accessible, and finally archived. Without an integrated data management solution these tasks are hardly to accomplish. Consequently, we have developed B-Fabric [1], a web-based data management system for supporting life sciences projects and integrating the produced data and needed applications.

B-Fabric is composed of loosely-coupled components based on open source technologies, such as PostgreSQL as database server for structured data, Lucene as full-text search engine, and ActiveMQ for asynchronous communication between the B-Fabric components. B-Fabric is available under Reciprocal Public License (RPL). For a description of the B-Fabric architecture and its underlying technologies, please check [2]. In this demo paper, we briefly mention the functionality B-Fabric provides at its interface and sketch some of the central features.

For the interpretation and reuse of experimental data, scientific annotations are crucial. Based on our experience with many bioinformaticians and researchers and their practical experiences and difficulties with using standard schemas MIAME or Gene Ontology, we decided to apply a concise metadata schema approach for B-Fabric.

All scientific data is organized in *projects*. Within a project, a user creates and generates data resources. A *data resource* is an abstraction of a file or link to a file. Examples for data resources are raw files produced from a mass spectrometer or cel files generated from an array scanner. Each data resource is connected to an *extract* representing the biological input into the experiment or measurement that produced the data resource. We distinguish between samples and extracts describing the biological sources at different levels. The *sample* contains general information about the biological source while the extract represents an extraction of that source

which actually is used for the experiment or measurement. There might be several extracts of one sample. These extracts might be the result of different extraction procedures.

As a result of extensive discussions between the bioinformaticians and researchers at FGCZ about the question what primary (and secondary) data should be stored and especially what this data actually represents, the generic concept of a workunit was found in B-Fabric. A *workunit* is an abstraction that can be used to represent the result of an experiment, a measurement, an analysis, a search etc. In principle, a workunit is a container referencing to data resources that logically form a unit. Some of these data resources are marked as input resources meaning that they were the inputs of the processing step (*application*) that created the remaining data resources. The scientist individually decides what a workunit should represent.

2 Use Cases

From a typical researcher's point of view, B-Fabric provides the following functionality:

- *Manage projects*: A researcher can add and remove users to or from his projects to allow or restrict access to data stored within the context of a project.
- *Register samples/extracts*: The researcher describes his biological sources as detailed as possible using an extensible vocabulary that is maintained and curated by experts (in our case by FGCZ employees). This support is basis for semantic enrichment of experimental data in a dynamic research environment as the FGCZ.
- *Import data*: The user selects an instrument from where he wants to import data. The user then selects the files and describes the workunit. Finally, the data resources are either linked or copied to B-Fabric while the user associates the data resources to extracts. This step is crucial for the correct interpretation and later reuse of the imported data especially by third parties when it become accessible after project publication.
- *Data browsing*: All core B-Fabric objects are bidirectionally linked together such that the user can easily browse through his/her data network.
- *Quick and advanced search*: A user may find relevant data using full-text search. A search may vary from certain attributes of certain objects to the content of readable attachments and data resources. This support is important as soon as the stored data sets become larger such that data browsing become apparently inefficient. Above that, it is needed for searching data of published projects.
- *Direct access*: Besides full-text search, there are direct links (shortcuts) to the core B-Fabric object classes, e.g. projects, samples, extracts, and workunits.
- *Data export*: A user may export the data in various ways, e.g., the entire workunit as a torrent file or as a report of a given template. Since the size of a workunit may be huge, B-Fabric creates a torrent file and provides it for download. For specific needs and applications, B-Fabric allows reports that collect and prepare data for later use.
- *Run external applications*: A user can invoke external applications with B-Fabric data. These applications are provided by experts who integrate them seamlessly into B-Fabric.

- *Open tasks*: B-Fabric shows the workflow tasks that the user has still to perform. This helps a lot to remember and softly force the user to terminate started workflows.

From a research center's point of view, B-Fabric additionally supports typical tasks that are crucial in efficiently running daily business in a such center:

- *Manage project*: To get access to the resource of the research center, e.g. using an instrument, a user needs to participate in a running project. B-Fabric supports the entire project management process, from the application submission over the reviewing to project member management. This feature is central for efficiently managing a core facility like FGCZ.
- *Register user*: Users themselves register and provide all personal contact information that is needed to grant access to the resources (computers, instruments etc.) of the research center. With the registration corresponding user accounts are generated such that the users can use all services with the same login and password. This frees the system admin from a lot of work.
- *Register external application*: A user with special access rights can couple external applications with B-Fabric such that these application can be invoked and fed via B-Fabric (for details see [3]). Based on some generic workflows and pageflows, a large bunch of applications can be added to the system on-the-fly. This feature is the basis for integrating already established data processing applications and pipelines into a common framework and extending the system's functionality in a loosely-coupled way. Experts can easily make new applications (written in any language and running anywhere) available to the whole user community. Depending on the type of data resources, B-Fabric provides the necessary invocation buttons and forms, respectively.
- *Merge Duplicates*: Some users tend to recreate a new user account due to various reasons. Eliminating such duplicates is the basis for an integrated view and analysis of a user's data and more importantly avoids unnecessary communication problems between a user and the staff of the research center. The duplicate merging is not only supporting for user information but also for other objects types like scientific annotations and institutional contact information.
- *Order (Door) Key*: A user that needs physical access to the userlab of the research center, requires a door key. Since B-Fabric maintains personal data of the users, ordering a door key at the university administration is a just one click away. This save a lot of time for the center's secretary as well as for the user.

3 Demonstration

In this demo paper, we sketch some central features of B-Fabric. As example scenario, we use a scientist who is working on a plant named *Arabidopsis Thaliana* with the goal to figure out the effect of certain gene and the effect on light on it. For this purpose, he registers his samples and extracts with B-Fabric, loads his data into B-Fabric and defines his experiment. Afterwards, he runs his experiment and stores the results in B-Fabric, as illustrated in Figure 1.

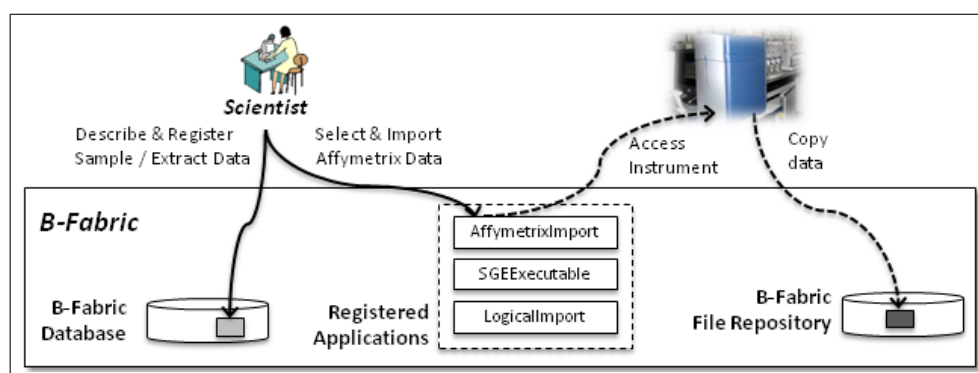


Figure 1: User runs Affymetrix Workflow

In the following, screen-shots are used to illustrate the different steps of the mentioned workflow. To avoid cluttering, the figures are clipped accordingly.

3.1 Register Samples/Extracts

Users register their samples and extracts through intuitively designed forms (see Figure 2 and 3). Data entering is facilitated by providing as much drop-down menus as possible to select annotations from the system vocabularies and by dynamically drawing forms according to selected annotation values.

The screenshot shows the **Edit Sample** form. It includes a header with a link to [The QuickGuide Proteomics / QuickGuide Transcriptomics](#) for registration information. The form fields are as follows:

- Name: dark_1_
- Project: 403 - Informatics Test Project
- Sample Type: Biological sample
- Species: 543 - Arabidopsis thaliana (thale cress)
- Strain: Columbia
- Sex: unisex
- Individual ID: 1
- Genotype: (empty)
- Genetic Modification: (empty)
- Disease State: Hopeless

Figure 2: Register Sample

In addition, users typically register several samples and extracts where only a few attributes differ. In order to further ease the registration, cloning as well as batch registration of samples and extracts are supported.

3.2 Data Import

B-Fabric supports two ways of data import: 1) physically copying and 2) linking data files. To import data from a data source, a proper data provider must be configured. In principle, data can be imported from any configured source that supports ssh for secure data transfer. The

Edit Extract

The [QuickGuide Proteomics](#) / [QuickGuide Transcriptomics](#) provide information about how to register an extract.

Name • dark_1_ ?

Project • 403 - Informatics Test Project ?

Parent Type • Sample ?

Parent Sample • 3289 - dark_1_ ?

Extract Type • Transcriptomics ?

Extraction Protocol • Select item ? +

Labeling Protocol • Affymetrix One-Cycle Target Labeling - Expression Arrays ? +

Figure 3: Register Extract

B-Fabric deployment at FGCZ allows importing data files from local file systems as well as several instruments available at FGCZ. New data providers can be added to the system easily. With the configuration of a data provider the selection of the data files in corresponding data stores can be restricted to the ones that are potentially relevant for the user. This is a crucial feature since the number of the data files can be huge. An import results in a workunit. Figure 4 shows the screen where a workunit is created by fetching files from the Affymetrix GeneChip instrument, which is an instrument already known to B-Fabric.

Create Workunit : Affymetrix GeneChip Import

A workunit is the container for all resources that are imported in one work step. This is the atomic unit for storing, annotating, searching and downloading data.

Name • Demo - LightStimulus Experiment Two Group Analysis ?

Project • 403 - Informatics Test Project ?

Description

Data Resources • Available (0)

Selected (6)

p403/Transcriptomics/Affymetrix/LightStimulus/caquinoof_20090312_dark_2_ATH1.CEL
 p403/Transcriptomics/Affymetrix/LightStimulus/caquinoof_20090312_sd1g_1_ATH1.CEL
 p403/Transcriptomics/Affymetrix/LightStimulus/caquinoof_20090312_sd1g_3_ATH1.CEL
 p403/Transcriptomics/Affymetrix/LightStimulus/caquinoof_20090313_dark_1_ATH1.CEL

Figure 4: Create Workunit

B-Fabric implements the data import via workflows. With the initiation of a data import, the corresponding workflow becomes visible to the user. The next step to be taken by the user is highlighted in the graphical representation of the workflow. In data import workflow, for instance, the user must assign extracts to the imported files. The workflow-driven approach of B-Fabric is very useful in practice to reduce human mistakes and avoid skipping steps.

Assigning extracts to data resources also comes with some intelligence in B-Fabric. When the scientist goes to the assign extracts screen, he gets already the best matches between data resources and extract names. Typically he just needs to press the save button and continue.

Figure 5: Assign Extracts

3.3 Application Integration

External functionality can be coupled with B-Fabric via *applications*. First, a connector is written for a certain type of application, e.g., for running *R* scripts on an *Rserve* system. Then, a small interface is defined to describe how the application gets its input (see Figure 6). Finally, the scientist writes the application in any language. This on-the-fly coupling of external applications is a crucial feature of B-Fabric, which allows fast extension and evolution of the system.

Figure 6: Application Registration

Once an application is registered, an experiment can be created to run this application. As an example, Figure 7 shows the definition of the experiment that will be conducted on the Arabidopsis Thaliana plant as mentioned earlier in this section. Defining an experiment consists of a selection of data resources, samples, extracts, and arbitrary number of attributes (e.g. species and treatment in the example.) that will be used as input for the application.

Figure 8 shows how easily a previously registered application (two group analysis) can be

Create Experiment Definition

Name: Demo - LightStimulus Experiment Two Group Analysis

Data Resource	Sample	Extract	Species	Treatment
p403/Transcriptomics/Aff	dark_1_	dark_1_	Arabidopsis thaliana (thali)	light deprivation
p403/Transcriptomics/Aff	dark_3_	dark_3_	Arabidopsis thaliana (thali)	light deprivation
p403/Transcriptomics/Aff	dark_2_	dark_2_	Arabidopsis thaliana (thali)	light deprivation
p403/Transcriptomics/Aff	sdlg_1_	sdlg_1_	Arabidopsis thaliana (thali)	light treatment
p403/Transcriptomics/Aff	sdlg_3_	sdlg_3_	Arabidopsis thaliana (thali)	light treatment
p403/Transcriptomics/Aff	sdlg_2_	sdlg_2_	Arabidopsis thaliana (thali)	light treatment

ADD ATTRIBUTE +

Figure 7: Create Experiment Definition

invoked to conduct the desired experiment. This step requires a name for the resulting workunit which contains the result files of the application along with specific parameters regarding the experiment, e.g. reference group.

Create Workunit : Two Group Analysis

Name: Demo - LightStimulus Experiment Two Group Analysis

Project: 403 - Informatics Test Project

Application: Two Group Analysis

Grouping: Treatment

Sample Group: light deprivation

Reference Group: light treatment

CDF Name:

Pairing: Select item

Run GO analysis:

Run MetaCore analysis:

Figure 8: Run Experiment

Once the experiment is started, a corresponding workflow is initiated. The graphic presentation of the workflow is also used to show what is happening underneath in the system. The example workflow (generate an R report) is quite simple and consists of a single step (see Figure 9). Note that B-Fabric can support arbitrary complex workflows based on its underlying workflow engine.

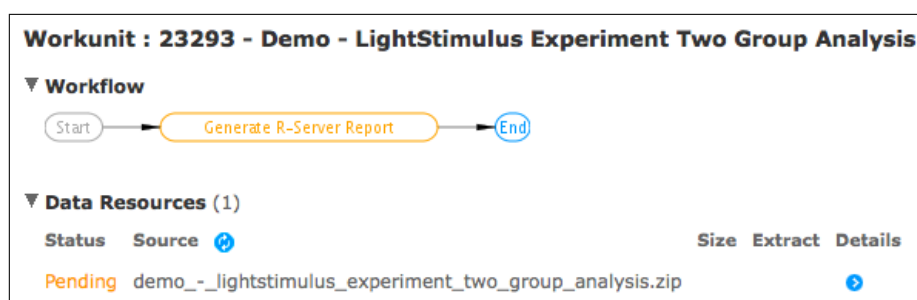


Figure 9: Run Experiment - Pending State

When the experiment is done, the scientist can view the experiment results by clicking the proper link on the screen (see Figure 10). The results of the experiment are also presented to the user as a zip file so that they can easily be transferred to another medium.

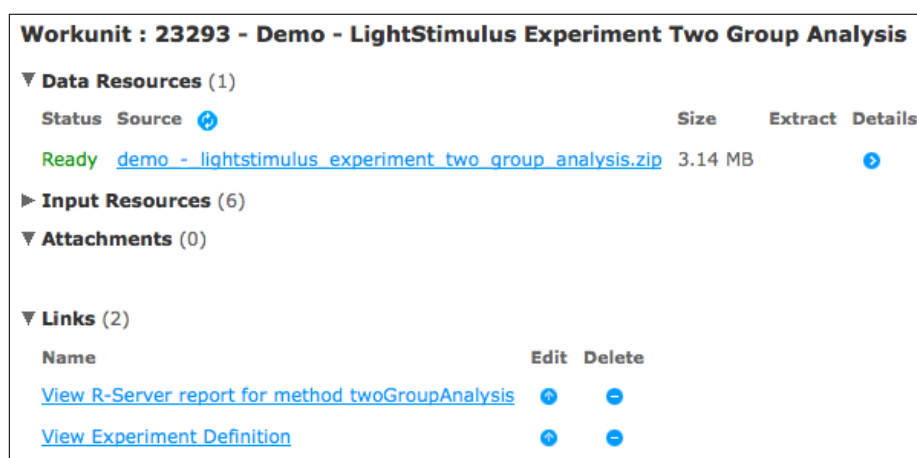


Figure 10: Run Experiment - Ready

4 Conclusions

B-Fabric is running in daily business at FGCZ since beginning of 2007. Here are some figures about the FGCZ deployment as of July 2011:

Users	2129	Projects	985	Samples	5917	Extracts	7708
Institutes	394	Organizations	98	Data Resources	84494	Workunits	54775

We now conclude this paper by sharing some experiences we made with running B-Fabric at FGCZ:

- Metadata Schema with Extensible Vocabulary.* In a very dynamic research environment as the FGCZ, it is practically impossible to agree on a schema that can capture all potentially created data in the application domain at a detailed level of granularity. Life science research data require two types of annotations in order to be able to interpret the contained information: (i) attributes describing the measurement parameters and (ii) attributes characterizing the biological samples measured. Both types cannot be well covered with a fixed annotation vocabulary. A life science data management system has to provide a flexible annotation scheme in order to be used at a center like the FGCZ that serves many different research fields.
- Physical and Logical Data Import.* To annotate experimental data, the system must first be aware of the corresponding files. Originally, B-Fabric was designed to move or copy all experimental data into its internal repository. Such a *physical* import is indispensable in scenarios where the data cannot be maintained persistently at the instrument PC or external data store for different reasons. However, a physical import into a fully encapsulated repository complicates the use and postprocessing of the data with typical analysis and visualization tools. Since such tools require direct access to the data files, the files must be downloaded, i.e. copied, to the corresponding places in the file system. Due to the size of the files and length of the scientific pipelines, this puts the researcher into an undesired long pending state. Hence, B-Fabric also supports a *logical* import (linking) of data such that the data files can reside at an external data store. Pre-configured data

