CABIG[™] SOFTWARE REQUIREMENTS AND SPECIFICATION

DOCUMENT CHANGE HISTORY

| Version Number | Date | Description |
|----------------|---------------|---------------------|
| 1.0 | November 2004 | Draft |
| 1.1 | March 2005 | Added Sign-Off Page |

Integrating Bioconductor and R into $caBIG^{TM}$ $Bioconductor / caBIG^{TM}$ Software Requirements and Specification Document $Version \ 1.0$

[Insert approval date of document]

Document Change Record

| Version Number | Date | Description | |
|----------------|-------------|--------------------------------|--|
| 1.0 | May 2006 | Draft | |
| 1.1 | June 2006 | VCDE comments | |
| 1.2 | July 2006 | Architecture, adopter comments | |
| 1.3 | August 2006 | Workspace comments | |

TABLE OF CONTENTS

| 1. | INT | RODUC | TION | 1 |
|----|------|--------|---------------------------------|-----|
| | 1.1 | SCOPE. | | 1 |
| | | 1.1.1 | Identification | 1 |
| | | 1.1.2 | System Overview | 1 |
| | | 1.1.3 | Document Overview | |
| | 1.2 | REFERE | ENCE DOCUMENTS | 2 |
| 2. | PRO | JECT D | DESCRIPTION | 2 |
| | 2.1 | PROJEC | T PERSPECTIVE | 2 |
| | 2.2 | | T FUNCTIONS | |
| | 2.3 | | HARACTERISTICS | |
| | 2.4 | | RAINTS | |
| | 2.5 | | TCATION PROVISIONS | |
| | 2.6 | | PTIONS AND DEPENDENCIES | |
| 3. | | | ENTS | |
| | 3.1 | | [™] REQUIREMENTS | |
| | | 3.1.1 | Vocabularies and data elements | |
| | | 3.1.2 | User Interface (UI) Guidelines | |
| | | 3.1.3 | API Access | |
| | | 3.1.4 | caGRID ACCESS | |
| | | 3.1.5 | Environment | |
| | 3.2 | | NALYTIC SERVICES (RWEBSERVICES) | |
| | 3.3 | | LAR FUNCTIONALITY | |
| | | 3.3.1 | Affy | |
| | | 3.3.2 | PROcess | |
| | | 3.3.3 | DNAcopy | |
| 4. | SYS' | | RCHITECTURE | |
| | 4.1 | | M ARCHITECTURE OVERVIEW | |
| | 4.2 | | ECTURAL DESIGN | |
| | 4.3 | | ACES | |
| | 4.4 | SYSTEN | 1 SECURITY | .11 |
| 5. | CON | MPONE | NTS | .11 |
| | 5.1 | RWEBS | ERVICES | .11 |
| | | 5.1.1 | <i>Type</i> | |
| | | 5.1.2 | Purpose | |
| | | 5.1.3 | Function | |
| | | 5.1.4 | Subordinate | |
| | | 5.1.5 | Dependencies | |
| | | 5.1.6 | Preconditions | |
| | | | Interfaces | |
| | | 5.1.8 | Resources | |
| | | 5.1.9 | References | |
| | | 5.1.10 | Processing | |
| | | 5.1.11 | Data | |
| | | 5.1.12 | Space estimates | |
| | | 5.1.13 | Impact to existing components | |
| | | 5.1.14 | System security | |
| 6. | | | | |
| | 6.1 | APPRO | VAL | .15 |

1. INTRODUCTION

This SRSD captures the complete software requirements for the $Bioconductor / caBIG^{TM}$ 1.0 release.

The purpose of this module is to provide tools to expose existing Bioconductor 'packages' as caGRID services.

1.1 SCOPE

Bioconductor is a collection of open-source software components based on the R programming language. Bioconductor is used for gene expression and other high-throughput analysis in molecular biology. R packages are collections of algorithms grouped to facilitate particular analyses.

This module allows R package developers to expose the functionality of their package as analytic services on caGRID. Operationally this will be performed at two different, but related, levels. One level is to expose Bioconductor packages on caGRID. A second level is to expose particular pipelines as 'exemplars'. Use cases outlining these goals are available¹.

The *primary concern* of this project is to develop tools for converting existing Bioconductor packages to caGRID analytic services. This is in contrast to other modules, which may focus on providing specific functionality as analytic services. This portion of the project involves development of software components to wrap functionality written in the R programming language as Java components, and to expose these Java components as analytic web services.

The *secondary concern* of this project is to expose particular Bioconductor pipelines as 'exemplars'. Exemplars are chosen from three Bioconductor packages. Candidate packages include *affy* (used for microarray analysis) *PROcess* (SELDI-TOF proteomics data) and *DNAcopy* (array CGH data).

1.1.1 Identification

 $Bioconductor / caBIG^{TM} 1.0.$

1.1.2 System Overview

The purpose of the system and software is to provide tools that facilitate developing existing Bioconductor packages as web services, exposure of web-services enabled packages as caGRID services, and discovery and invocation of web-services enabled packages as caGRID analytic services.

The tools in $Bioconductor / caBIG^{TM}$ 1.0 represent new software development, sponsored by the National Cancer Institute through the cancer Biomedical Informatics Grid (caBIGTM). End users include caBIGTM participants, as well as members of the public. Module development is

 $^{^1\} http://cabigcvs.nci.nih.gov/viewcvs/viewcvs.cgi/bioconductor/Administrative Deliverables/Use_Case.pdf$

conducted at the Fred Hutchinson Cancer Research Center in Seattle, WA, under the overall direction of Dr. Robert Gentleman.

Software developed in this project will be installed and used at our caBIGTM adopter sites (Northwestern University) and will be available for installation and use at other caGrid locations.

1.1.3 Document Overview

This SRSD captures the complete software requirements for $Bioconductor / caBIG^{TM}$ 1.0 as part of the $Integrating\ Bioconductor\ and\ R\ into\ caBIG^{TM}$ project.

There are no security or privacy considerations directly associated with use of this software. However, software underlying the project cannot be considered secure; security must be provided by other caGRID software layers.

Software developed specifically for this project is licensed under caBIGTM licensing terms. The underlying R software is open source and licensed under the GPL version 2. Additional license restrictions apply to individual Bioconductor packages.

The remaining SRSD sections are organized as follows:

- **Section 2. Project Description**: Describes the general factors that affect *Bioconductor* / $caBIG^{TM}$ 1.0
- **Section 3. Requirements**: Describes all the software requirements to a level of detail sufficient to enable designers to design a system to satisfy those requirements, and testers to test that the system satisfies those requirements.
- Appendix A. Acronym List: Defines the abbreviations used on the project.

1.2 REFERENCE DOCUMENTS

For additional project and requirement specific information, please consult the administrative deliverables and documentation available at:

 http://gforge.nci.nih.gov/plugins/scmcvs/cvsweb.php/bioconductor/Developer_FHCC/?cvsro ot=bioconductor

2. PROJECT DESCRIPTION

2.1 PROJECT PERSPECTIVE

The main software component to be produced by this project is the RWebServices package. In broad terms, the software is a collaboration between three R packages (TypeInfo, RWebServices [to be developed here], and SJava) to allow R functions to be wrapped as Java classes. Script and other caCORE and caGRID methodologies (incorporating existing technologies, augmented with documentation and development here) transform the Java classes to caGRID-enabled components. Additional facilities provided by the RWebServices package facilitate invocation of Bioconductor functions as caGRID analytic services.

The delivery platform being targeted is a current linux operating system capable of caGRID service; this does not preclude deployment on Windows operating systems. Specific constraints are listed below.

2.2 PROJECT FUNCTIONS

TypeInfo (a previously developed product) is an R package to provide strong typing and introspection on function argument and return types. TypeInfo is used to annotate functions in existing Bioconductor packages, and is a necessary first step in making the functions available as web services.

RWebServices is to be developed here as an R package (with some C code) that produces Java beans encapsulating the function and data type signatures of TypeInfo-annotated functions. The package uses type specification and R introspection facilities to determine the underlying data structure of R objects. The data structure is then translated into a corresponding Java class representation.

RWebServices also facilitates analytic service invocation. It does so by including in automatically generated Java classes the methods required for invoking an R evaluator and calling appropriate R functions from Java, and by providing native translation services between Java objects and their R representation.

SJava is an existing technology consisting of R, Java, and C code. It allows R functions to be called from Java, and vice versa. SJava recognizes Java class objects, and translates data represented in Java classes to their corresponding R representation. Data translation occurs at the C level. The Java classes produced by RWebServices are fully interoperable with SJava.

To be available as caGRID analytic services, standard web services require semantic annotation. The tools required for semantic annotation are not a software product of the current project but are provided by the caCORE SDK.

Installation of appropriate modified Bioconductor packages as caGRID analytic services involves steps identical to those required to install any collection of Java objects as analytic services, so the tools required for this step are not a software product of the current project. Steps specific to installing Bioconductor packages as web services will be documented; scripts or other functionality to automate specific steps in this process (e.g., coordinating installation of Bioconductor packages, their Java representation, and semantic annotation information) will be developed.

Invocation of Bioconductor functionality as an analytic service requires correct installation of R, Bioconductor, and SJava, in addition to standard requirements for caGRID analytic services. Our project will document recommended ways of installing R, Bioconductor, and SJava, and will provide installation software to automate this process, as appropriate.

2.3 USER CHARACTERISTICS

Primary users of this software include Bioconductor package developers and caGRID node administrators. A secondary user is the individual invoking Bioconductor functionality as an analytic service.

The Bioconductor package developer is computationally- and statistically capable individual wishing to produce or modify an R package to be deployed as an analytic service in caGRID. The individual is familiar with R, but has no special skills related to analytic services. The individual needs to be informed of the steps required for function and data type specification, and for producing Java classes corresponding to their Bioconductor package.

The caGRID node administrator is familiar with caGRID architecture and semantic annotation requirements of caCORE. The role of the administrator is to facilitate semantic annotation, and to install and deploy Bioconductor packages as web services. This individual may have limited familiarity with R, requiring that installation steps unique to R be documented.

2.4 CONSTRAINTS

- a. Architecture. Our project is directed toward a current linux operating system with standard development tools. These tools include those² required to build R. The system has versions of Java required for SJava³ and caBIG^{TM 4}. Deployment and invocation tools require the web service infrastructure specified by caGRID⁵. Extension to use on Windows requires installation of specific but readily available software tools for R development, as indicated in footnote 2; Java and caGRID requirements on this platform are detailed in the documents cited earlier.
- b. Data standards. Bioconductor packages analyze a diversity of data types; ensuring that these correspond to existing data types accessible as caGRID data services is the responsibility of individual package developers.
 - Analytic services frequently have 'tuning' and other parameters required for function evaluation but largely irrelevant to semantic interoperability. Tuning parameters will be represented as semantically annotated objects, as required by caBIO.
- c. Programming language versions. R packages developed during this project will require the R-2.4.0. Requirements on Java are those specified by caGRID.

2.5 QUALIFICATION PROVISIONS

a. Specific code-based test facilities will be constructed to qualify requirements 3.1.*, 3.2.*, and 3.3.* (* represents all subsections).

2.6 ASSUMPTIONS AND DEPENDENCIES

This project relies on services provided by caDSR (curate data types) and caGRID (analytic service infrastructure).

⁵ https://cabig.nci.nih.gov/workspaces/Architecture/caGrid

_

² http://cran.r-project.org/doc/manuals/R-admin.html

³ http://www.omegahat.org/RSJava/

⁴ https://cabig.nci.nih.gov/

3. REQUIREMENTS

There are three requirement types indicated below. Requirements for caBIGTM are presented first. The RWebServices component is a software unit responsible for particular functionality. 'Exemplars' are specific Bioconductor functionality to be exposed as proof-of-methodology.

3.1 CABIG[™] REQUIREMENTS

This section describes the requirements for this release in order to achieve caBIGTM Silver compatibility.

3.1.1 Vocabularies and data elements

One of the main goals of caBIGTM is to ensure that all applications use the same vocabulary and data elements for similar concepts across the grid. This is aimed at eliminating inconsistency in data descriptors (metadata) and hence makes it possible to pass semantically equivalent data with confidence across various applications within the grid.

| Req ID | Require ment Type | Requirement Description | CCR # (Optional) | Trace from User Requirement/ Trace to System Requirement (Optional) |
|---------|-------------------------|---|---------------------|---|
| 3.1.1.1 | caDSR Usage | Bioconductor / caBIG TM must use the Cancer Data Standards Repository (caDSR) and Enterprise Vocabulary Services (EVS) for each data element and concept that will be exposed to the grid. | | |

3.1.2 User Interface (UI) Guidelines

As an analytic web service, Bioconductor / $caBIG^{TM}$ does not have a graphical UI.

3.1.3 API Access

The main goal of caBIGTM is to create a network or grid of applications, tools, and data, thereby creating a *World Wide Web* of cancer research. In order to achieve this, all silver-compliant caBIGTM applications must provide an Application Program Interface (API) so that others can retrieve meaningful data, correlate data with other applications, or create new applications.

| Req ID | Requirement Type | Requirement Description | CCR # (Optional) | Trace from User Requirement/ Trace to System Requirement (Optional) |
|---------|---------------------|--|---------------------|---|
| 3.1.3.1 | API Access | Bioconductor / caBIG TM must provide caCORE like APIs to expose functionality as an analytic service. | | |

3.1.4 caGRID ACCESS

All gold-compliant caBIGTM applications must act as data and/or analytical services on the caGRID so that others can retrieve and/or analyze meaningful data, correlate data with other applications, or create new applications.

Bioconductor / caBIGTM is funded for silver compatibility, and does not have requirements for caGRID access. Nonetheless, our intention is to provide caGRID enabled analytic services.

| Req ID | Requirement Type | Requirement Description | CCR # (Optional) | Trace from User Requirement/ Trace to System Requirement (Optional) |
|---------|---------------------|--|---------------------|---|
| 3.1.4.1 | caGRID Access | Bioconductor / caBIG TM must be caGRID enabled and act as a data and/or analytical service on caGRID. | | |

3.1.5 Environment

All caBIGTM projects should be platform- and database-independent applications. This means that it should be possible to run Bioconductor / caBIGTM on any operating system. Considering the large number of combinations of test scenarios, however, Bioconductor / caBIGTM must be certified for the environments listed in Table 1.

Table 1: System configurations for Bioconductor / caBIGTM

| Server operating system | Suse 10.0 |
|-----------------------------------|----------------------------|
| Apache, Tomcat, Globus, Java, ant | As specified by caGRID 1.0 |
| R | 2.4.0 |
| SJava | 0.6-4 |

3.2 R AS ANALYTIC SERVICES (RWEBSERVICES)

RWebServices is required to construct Java classes corresponding to S4 or core R data types and Java function signatures based on R functions annotated by TypeInfo. RWebServices constructs methods for dispatch of analytic services from Java to R. RWebServices augments SJava native translation between Java and R.

| Req ID | Requirement Type | Requirement Description | CCR # (Optional) | Trace from User Requirement/ Trace to System Requirement (Optional) |
|-----------|---------------------|---|---------------------|--|
| 3.3.1 | Component | Produce Java classes corresponding to S4 or core R data types | | |
| 3.3.2 | Component | Produce Java classes encapsulating equivalent | | |

| | | R function signature(s) | |
|-------|-----------|---|--|
| 3.3.3 | Component | Provide methods to dispatch analytic services for R evaluation | |
| 3.3.4 | Component | Provide (in conjunction with SJava) data translation services between Java and R internal representations of core R data types. | |
| 3.3.5 | Component | Provide error reporting functionality associated with R function evaluation. | |
| 3.3.6 | Component | Correctly return R results as Java data objects to analytic service requests. | |

3.3 EXEMPLAR FUNCTIONALITY

Our tools enable annotation and publication of Bioconductor packages as analytic services, rather than wholesale conversion of Bioconductor packages for this purpose. Nonetheless, our project includes exemplars chosen from three different areas of Bioconductor functionality. The goal is to expose at least one function from each package as a caGRID analytic service.

3.3.1 Affy

The package contains functions for exploratory oligonucleotide array analysis. Functionality includes background correction, normalization, and expression summaries. Inputs are typically collections of microarray expression values representing data collected from several samples in a single experiment. Outputs are typically transformed expression values or summary presentations. The MAGE-OM⁶ is used where possible.

| Req ID | Requirement Type | Requirement Description | CCR # (Optional) | Trace from User Requirement/ Trace to System Requirement (Optional) |
|---------|---------------------|---|---------------------|---|
| 3.3.1.1 | Exemplar | Expose specific functionality as a web service, using TypeInfo, RWebServices, and SJava. Exposed data elements are associated CDEs. | | |
| 3.3.1.2 | Exemplar | Receive MAGE-OM object | | |
| 3.3.1.3 | Exemplar | Invoke and perform analytic service corresponding to the 'expresso' function in the 'affy' package | | |
| 3.3.1.4 | Exemplar | Add resulting transformation and documentation to MAGE-OM object | | |
| 3.3.1.5 | Exemplar | Return transformed MAGE-OM object from web service. | | |
| 3.3.1.6 | Exemplar | Report errors during execution | | |
| 3.3.1.7 | Exemplar | Satisfy silver-level compatibility requirements | | |

 $^{^6\} http://www.mged.org/Workgroups/MAGE/mage-om.html$

3.3.2 PROcess

PROcess is a package for processing protein mass spectrometry data. Functionality includes baseline subtraction, peak identification, and quality control. Inputs are typically collections of SELDI-TOF mass spec scans representing data from a single experiment. Outputs are typically transformed scans, peak identification vectors, or summary presentations. The mzXML domain model⁷ is used where possible (for input parameters)

| Req ID | Requirement Type | Requirement Description | CCR # (Optional) | Trace from User Requirement/ Trace to System Requirement (Optional) |
|---------|---------------------|--|---------------------|--|
| 3.3.2.1 | Exemplar | Expose specific functionality as a web service, using TypeInfo, RWebServices, and SJava. Exposed data elements with associated CDEs. | | |
| 3.3.2.2 | Exemplar | Receive mzXML object | | |
| 3.3.2.3 | Exemplar | Invoke and perform analytic service, reporting correct result to user | | |
| 3.3.2.4 | Exemplar | Return aligned peaks in a CDE-defined data structure. | | |
| 3.3.2.5 | Exemplar | Report errors during execution | | |
| 3.3.2.6 | Exemplar | Satisfy silver-level compatibility requirements | | |

3.3.3 DNAcopy

DNAcopy segments DNA copy number data collected from array CGH experiments, using circular binary segmentation to detect regions with abnormal copy number. Functionality includes smoothing and segmenting copy number data. Typical inputs are vectors corresponding to marker location and sample copy numbers. Outputs are vectors of sample identifiers, segment start and stop positions, and related statistics.

| Req ID | Requirement Type | Requirement Description | CCR # (Optional) | Trace from User Requirement/ Trace to System Requirement (Optional) |
|---------|---------------------|--|---------------------|---|
| 3.3.3.1 | Exemplar | Expose specific functionality as a web service, using TypeInfo, RWebServices, and SJava. Exposed data elements with associated CDEs. | | |
| 3.3.2.2 | Exemplar | Receive CDE-defined data object representing raw DNA copy number data. | | |
| 3.3.2.3 | Exemplar | Invoke and perform analytic service, reporting correct result to user | | |
| 3.3.2.4 | Exemplar | Return CDE-defined data object describing marker location and copy number. | | |
| 3.3.2.5 | Exemplar | Report errors during execution | | |
| 3.3.2.6 | Exemplar | Satisfy silver-level compatibility requirements | | |

4. SYSTEM ARCHITECTURE

⁷ http://tools.proteomecenter.org/mzXMLschema.php

4.1 SYSTEM ARCHITECTURE OVERVIEW

The high-level concept of the system is the development and exposure of R functionality as web services for statistical analysis of high-throughput biological data. In general the statistical methodologies are previously defined, and their specification is outside the scope of this document. The focus here is on two main aspects of the project: service creation from existing analytic functionality, and service evaluation in the caGRID services environment.

Statistical analytic routines are existing functions written in the R programming language and distributed as R libraries. Extensive documentation of the R programming language is available⁸, as are details of the analytic functionality available in existing R / Bioconductor packages⁹.

The system architecture for service creation consists of an existing Bioconductor package (e.g., affy, PROcess, or DNAcopy, above) coupled with the R libraries TypeInfo (previously developed) and RWebServices (to be developed here). The architecture relies on user access to simple text file creation utilities, a command line environment, and system software requirements for the R user environment. In general, R runs on modern linux, MacOS, and Windows desktop or server computers with standard software tools.

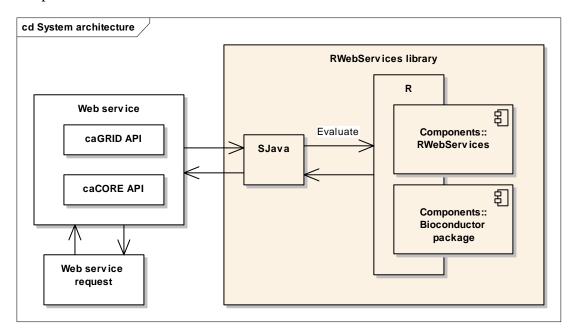


Figure 1 System architecture block diagram – service invocation. Tan objects represent components provided by Bioconductor / $caBIG^{TM}$.

The system architecture for service invocation consists of an established caGRID node with installed Java. Software components provided by this project include SJava, R, Bioconductor package(s), and the RWebServices package.

⁹ http://bioconductor.org

⁸ http://cran.fhcrc.org

Safety, security, and privacy design decisions are under the purview of caGRID services.

4.2 ARCHITECTURAL DESIGN

For analytic service creation, the basic control and data flow starts with an existing Bioconductor package and a TypeInfo annotation file identifying functionality, argument, and return types to be exposed from the package as web services. The package and TypeInfo annotation file are processed by TypeInfo and RWebServices to create a hierarchy of Java data class objects with data element accessor methods, and a Java class with Bioconductor functionality exposed as strongly typed Java functions. An additional Java class coordinates the requests for analytic services with the R evaluator. The Java data elements and functionality are semantically annotated using caCORE SDK. The semantically annotated functionality is exposed as a grid analytic service using the caGRID SDK. This work flow is documented in detail in the Bioconductor Use Case document¹⁰; the architectural design of the caCORE and caGRID SDKs are outside the scope of this document.

The remaining paragraphs in this section refer to software units participating in analytic service invocation, and diagramed in Figure 1.

The component labeled 'web service' represents caBIGTM infrastructure outside the scope of this document. In the context of the present project, the resource use of this infrastructure is likely to involve substantial data transfer bandwidth (data files of 10's-100's of MB) and corresponding memory.

R and Bioconductor are existing software packages for statistical computation. Extensive documentation of the R programming language is available 11 , as are details of the analytic functionality available in existing R / Bioconductor packages 12 .

SJava is an existing software package that embeds R in a Java environment. The purpose of SJava in our implementation is as an interface between caGRID and R. The requirement placed on SJava for the present project is native translation between web services and R representations of data objects, and the ability to invoke R functions from Java. The current version of SJava is 0.69-4. Documentation for SJava is available¹³.

RWebServices is a component of R. Its function in the context of service invocation is to correctly construct Java methods for dispatch of analytic service requests to R functions, and to extend native SJava data translation between Java and R. RWebServices is currently in development. It has minimal resource use requirements beyond those of R.

 $http://gforge.nci.nih.gov/plugins/scmcvs/cvsweb.php/bioconductor/Developer_FHCC/Task\%202.2.2_Final\%20Use\%20Case\%20Document/Use_Case.doc?cvsroot=bioconductor$

¹⁰

¹¹ http://cran.fhcrc.org

¹² http://bioconductor.org

¹³ http://www.omegahat.org/RSJava/

Exemplar packages are components of R. Packages provide analytic service evaluation, as detailed in section 3.3. Analytic components of packages are fully developed. Interfaces consistent with caBIGTM requirements are under development. Resource use is highly variable depending on service request. Typical memory requirements are 1-2GB with computation times of 1-2 minutes on systems outlined above.

4.3 INTERFACES

The primary interface to Bioconductor / caBIGTM is as caGRID service.

- External Software Interfaces Bioconductor / caBIGTM interfaces with caGRID as an analytic service. The interface requirements are as specified by caGRID.
- \bullet Software System Interfaces There are no special system software interfaces required for Bioconductor / caBIGTM.
- Software System Components Interfaces Interfaces between RWebServices and SJava are outlined below; there are no additional system software component interfaces.
- Hardware Interfaces There are no hardware interfaces beyond those required by caGRID.

4.4 SYSTEM SECURITY

- Network Level Bioconductor / caBIGTM relies on network security provided by the caGRID infrastructure.
- Database Level There are no database-level system security issues.
- Application Level Application level security is facilitated by independent R function evaluation and no persistent data caching for each requests.

5. COMPONENTS

5.1 RWEBSERVICES

5.1.1 Type

R package.

5.1.2 Purpose

The purpose of this component is to provide a Java interface to existing Bioconductor functions, as specified in requirement section 3.2.

5.1.3 Function

The component has two distinct functionalities.

During analytic service creation, RWebServices transforms a list of TypeInfo-annotated functions to a hierarchy of Java data classes (corresponding to the R S4 types indicated by TypeInfo) and methods for evaluating functions.

During analytic service invocation, classes created by RWebServices dispatch analytic service requests for evaluation in R. RWebServices also provides native bidirectional translation between Java objects and their corresponding R S4 classes.

5.1.4 Subordinate

None.

5.1.5 Dependencies

RWebServices depends on TypeInfo during analytic service creation, and SJava during service invocation.

5.1.6 Preconditions

RWebServices requires existing Bioconductor packages with functions containing TypeInfo attributes. During invocation as an analytic service RWebServices requires caGRID infrastructure to correctly specify data elements and functions and SJava methods for R evaluation.

5.1.7 Interfaces

5.1.7.1 Analytic service creation

RWebServices takes as input a list of TypeInfo-annotated functions. It produces as output a hierarchically-arranged collection of Java data and function classes. Each Java data class contains private members corresponding to the data elements of the corresponding S4 object. There are public methods to 'get' and 'set' each data element.. The hierarchy localizes data definitions to folders specific to the R library in which the data or function was specified, e.g., bioc.affy.function.expresso.

RWebServices has access to the R libraries where the function is originally defined, and where data objects referenced by the type information attributes are defined.

5.1.7.2 Analytic service invocation

Classes created by RWebServices provide an interface between analytic services and R function invocation. The interface exposed as analytic service consists of a function name and strongly-typed argument and return values. The interface is augmented by semantic annotation services provided by the caCORE SDK.

The interface to RWebServices during analytic service invocation also follows the requirements and specifications of SJava. Specifically, RWebServices contains C-level converter functions that augment SJava functionality. The C-level converter functions accept and return the R SEXP data structure. Translation services provided by RWebServices in both directions is performed on the R, rather than Java, side of the bridge.

5.1.8 Resources

Not applicable.

5.1.9 References

Online and package documentation of the SJava interface is available ¹⁴.

5.1.10 Processing

5.1.10.1 Analytic service creation

R pseudo-code for the overall functionality of analytic service creation is as follows:

Function creation pseudo-code is:

```
buildRWebServicesInterface <- function(jTypeInfoByPkg) {
   rGlobalClass <- createOrGetGlobalEnv() # global wrapper for R functions
   for (pkg in jTypeInfoByPkg) { # each package separately
      jClass <- createRWebServicesInterfaceTemplate() # template
      for (funcs in pkg) {
        addInterfaceMethod(jClass, funcs) # interface to R wrappers
        addWrapper(rGlobalClass, funcs) # wrappers to R</pre>
```

¹⁴ http://www.omegahat.org/RSJava/

```
}
    writeJClass(pkg, jClass) # save to disk
}
writeRGlobalClass(rGlobalClass) # save / update global wrapper
}
```

5.1.10.2 Analytic service invocation

Service requests arrive and are decoded by caGrid functionality. The service request is then dealt with by the following pseudo-code:

```
rws = RWebServicesServ(); // Start R evaluator, load R libraries and converters, etc
try {
         result = rws.analyticService(serviceArgs); // invoke service with args
} catch (java.rmi.RemoteException e) {
         reportException(e);
}
return result;
// rws terminates R evaluator when out of scope
```

The .analyticService invokes a method in rGlobalClass to call and evaluate, through SJava, the R function. The returned result is packaged and forwarded to the requesting service by caGRID.

Program flow for each data translation function is straight-forward: create a new instance of the target object corresponding to the source object, populate the target object with source data, and return the target object. Populating the target object with data typically involves a memory copy.

There are no provisions for user interrupts; this is not a usual part of the web services workflow.

5.1.11 Data

There are three types of data internal to this component. R objects are represented as Java data classes, typically with a structure:

```
public class RClass extends rtypes.RObject {
    private rtypes.RNumeric eps; // data slot
    public RClass () {} // creation
    public void setEps(rtypes.RNumeric eps) {...} // set
    public rtypes.RNumeric getEps() {...} // get
    public String toString() {...} // string representation, for debugging / testing
}

Java function interfaces are structured as

package biocJavaMap.RWebServicesServ;
import org.omegahat.R.Java.ROmegahatInterpreter;
import org.omegahat.R.Java.REvaluator;
import java.util.*;

public class RWebServicesServ {
    private REvaluator e; // local evaluator
    private biocJavaMap.rGlobalEnv.function.rGlobalEnv myrGlobalEnv;

    public RWebServicesServ() throws Exception {...} // creation
    public rtypes.RNumeric rGlobalEnv_RFuncl(funcArgs1) {...} // invocation
```

}

package biocJavaMap.rGlobalEnv.data;

public rtypes.RNumeric rGlobalEnv_RFunc2(funcArgs2) {...} // invocation

The R function wrappers are in a rGlobalEnv data structure:

SJava defines the REvaluator object.

5.1.12 Space estimates

Space estimates for internal data objects are minimal. Run-time space estimates for data objects can be large (1-2GB), depending on data sizes of service requests.

5.1.13 Impact to existing components

Not applicable

5.1.14 System security

Application-level security is determined by the Java runtime environment. Embedded R inherits application-level security from Java, but R does not have a robust security model. Separate invocation of the R evaluator for each service request ensures that data does not persist between service invocations.

6. SIGN OFF

6.1 APPROVAL

| Architecture Workspace Rep | Print Name | Date |
|----------------------------|------------|------|
| VCDE Workspace Rep | Print Name | Date |
| Adopter Rep | Print Name | Date |

APPENDIX A - ACRONYM LIST

| Term/ Abbreviation | Description |
|-----------------------|------------------------------------|
| DBA | Database Administrator |
| PM | Project Manager |
| RM | Requirements Manager |
| RTM | Requirements Traceability Matrix |
| SCM | Software Configuration Management |
| SDLC | Software Development Lifecycle |
| SDP | Software Development Plan |
| SE | Software Engineering |
| SEPG | Software Engineering Process Group |
| SM | Software Manager |
| SOP | Standard Operating Procedure |
| SPI | Software Process Improvement |
| SQA | Software Quality Assurance |
| SW | Software |
| TBD | To Be Determined |
| TM | Test Manager |