Java VAMDC-TAP Node software

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Abstract: This document is a guide for the installation and use of the Java VAMDC-TAP Node software implementation.

Version History

Version	Date	Modified By	Description of Change
V0.1	31/10/2011	M.Doronin	first draft
V12.07	29/08/2012	M.Doronin	Release documentation for 12.07 Java node software
V12.07r2	28/10/2015	M.Doronin	Updates for 12.07r2 release of the Java Node Software

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CONTENTS

CHAPTER

ONE

PREFACE

This document describes the implementation and installation of a VAMDC-TAP node using the Java Node Software. It is organized to follow the node development path. Each chapter corresponds to an individual development task.

In the *Introduction*, a brief description of the components employed in the java node software implementation is given.

Node architecture chapter presents the architecture of the Java Node Software and gives the details on the interaction interfaces between the node software parts.

Setting up the development environment with the TAPValidator program is described in the *Database plugin testing* chapter.

The first development task is to access the data in the database. Apache Cayenne library is used to perform this task. The process is briefly described in the chapter *Database Object Model*. Once the access to the data is established, one may proceed to building the XSAMS elements from the database objects, as described in the chapter *XSAMS tree building*. The last development task is to define the mapping between the incoming VSS2 queries and the internal database queries. The chapter *VSS query parsing and mapping* describes that mapping in detail.

By this moment, node plugin should be capable of producing the XSAMS documents in response to incoming queries. Final development task is to implement special queries used to estimate if the database contains data for a given VSS2 request. It is described in the *Query metrics support* chapter.

The last chapter and last task is to install the node web service (*VAMDC-TAP node deployment*).

CHAPTER

TWO

WEB-SERVICE DESCRIPTION

Java implementation of VAMDC-TAP node software is a web-service application implementing a RESTful interface according to VAMDC-TAP standard specification.

It is accessible using the HTTP protocol, with URLs like *http://node.name.tld/vamdc-tap/12_07/VOSI/capabilities* or *http://node.name.tld/vamdc-tap/12_07/TAP/sync?query=select%20species&lang=VSS2&format=XSAMS*. Here *http://node.name.tld/vamdc-tap/12_07/* is the node base url, **/VOSI/capabilities** and **/TAP/sync** are endpoint addresses, and *?query=select%20species&lang=VSS2&format=XSAMS* are HTTP request parameters.

2.1 Web-service endpoints

Java implementation of VAMDC-TAP node software implements the following webservice endpoints:

- /VOSI/capabilities Virtual Observatory Support Interface - service capabilities endpoint. Reports the service capabilities and available IVOA and VAMDC-TAP addresses, as well as their mirrors. Accept no parameters.
- /VOSI/availability Virtual Observatory Support Interface - service availability endpoint. Reports the service availability and internal checks status. Accepts no parameters.
- /TAP/sync VAMDC-TAP synchronous query interface, accepting HEAD and GET requests. Mandatory parameters are **query**, **lang** and **request**. Refer to the VAMDC-TAP standard documentation for more details.
- /config Returns the web-service configuration options
- /clear_cache Forces the purge of Apache Cayenne object caches. May be called on the database update to force the node software to reload the data from the database.

CHAPTER

THREE

INTRODUCTION

Java implementation of the VAMDC-TAP node software was created in parallel with the Python version to pursue several objectives:

- Insure that standards are complete and contain no implementation-specific elements
- Give a choice of an implementation to node maintainers
- Employ the schema-based DOM XML generator to ensure the document validity. It presents an alternative approach to the keywords dictionary as used in Python/Django node software - see below the *Differencies* section

3.1 Used software

The following open-source libraries and components are used:

- JAXB Reference Implementation (RI) for XML schema mapping and XSAMS document output
- Apache Cayenne ORM framework for database access
- MySQL database (any relational database can be used via Apache Cayenne)
- ANTLR generated query parser with slightly modified SQLite syntax to transform the incoming query into the tree of objects
- Oracle Jersey JAX-RS implementation to support the VAMDC-TAP webservice interfaces
- Apache Tomcat application server to run the Java VAMDC-TAP web application

3.2 VAMDC common components

Additional libraries were developed within the VAMDC project are part of Java VAMDC-TAP node software.

- **Dictionaries of standard keywords,** used in a query;
- **Query parsing library,** providing object-oriented view on a query string;
- **Query mapping library,** providing basic support for mapping of incoming queries to the node database queries using Apache Cayenne objects.
- **XSAMS helper library,** providing convenience methods for output XML generator implementation;
- **Web application,** .war archive integrating all libraries
- **TAPValidator,** VAMDC-TAP service validation tool that may be used for node plugin testing on all phases of development.

3.3 Node-specific components

In Java node software each node installation requires creating two libraries:

1. **Database Access Objects using Apache Cayenne.** This task is well described in the Apache Cayenne documentation [CAYDOC] . A graphical tool is provided allowing to define the database structure and relations. Java classes corresponding to table entities are generated using this tool.
2. **Node plugin,** A piece of software that implements the node plugin interfaces and integrates with Java VAMDC Node Software application. Node plugin is responsible for a query translation into the database-specific queries and for building the appropriate XSAMS tree from the fetched database access objects.

3.4 Comparison with the python/django node software

The paragraph provides a comparison between the Java-Implementation and the Python/Django node software

3.4.1 Common features

Both Java and Python node software implementations

- Work as a web application behind a web server
- Use object-relational mapping to access the database
- Provide the implementation of the parts that are common for all nodes
- Node-specific part works as a plugin, that means that no modification to the common components is needed during the node-specific part development.

3.4.2 Differencies

- **The main architectural difference** between the the Java implementation and the Python/Django one is the XML generator.

  Java version uses Document Object Model (DOM) mapping of the XML, Java node plugin needs to build XSAMS blocks as trees of objects.

  Python/Django version provides the XML generator with a defined and limited set of loops and anchors(“returnables”). Node developer needs to study not only the XSAMS documentation, but also to look through a plane list of keywords to correctly pin the data to the XML document structure.

  The use of DOM XML mapping has some advantages and disadvantages:

  – On a positive side, it gives more flexibility for the document generation. Any attribute of the output document can be accessed

and set without the XML generator modification.

- The output document is kept error-free because of the compile-time type checks and runtime XML special symbols filtering.
- XML DOM mapping provided is complete: even if node developer wishes to put the data in a rarely used element of XSAMS, he can do it without the need to output XML blocks as the plain text.
- On a bad side, the task of building a document tree requires an additional amount of node-specific code. Parts of XSAMS-extra library provide helper methods to simplify this task.
- Memory consumption is higher due to the need to keep the whole document tree in memory.

- Document output is started after the construction of the XML tree, an additional delay is introduced, compared to the immediate streaming of the output by the Python/Django node software.

For the task of implementing XSAMS blocks builder, existing builders of KIDA, BASECOL and VALD may be used as examples.

- **Java implementation does not support document streaming.** The whole document tree is built in memory before producing the output XSAMS response.

  This approach allows to generate the document in the arbitrary order, i.e. export some species and states, then export processes, while exporting some more species and states.

- Java implementation does not provide any import tool from ASCII files into a relational database

  The node developer is himself responsible for creating and maintaining the node database structure and administration tool.

- Java implementation provides a sophisticated query parsing and mapping support

3.5 Node implementation

Implementing a node with the Java Node Software would require the following steps:

- The database model and classes should be created, as described in the *Database Object Model* section.

  After completing this step you will be able to access your database in a convenient way from any Java software you develop. For the details, see the Apache Cayenne documentation. [CAYDOC]

- The development environment for the plugin should be deployed. The query process and the interaction of the node and the plugin should be understood. See the *Node architecture* section for the details.

- XSAMS tree builders should be created, as described in the *XSAMS tree building* section. This work should be performed in collaboration with a person responsible for the scientific content of the database to establish the correspondance of the XSAMS elements and the database content.

  At this step the node plugin may be tested according to the procedure described in the section *Database plugin testing*. XSAMS generation should be verified and all the validation errors should be eliminated at this step.

- The supported restrictables and corresponding mappings should be defined, as described in the *VSS query parsing and mapping* section.

  Once this step is accomplished, it becomes possible to send different queries to the node. It should be checked if all the produced XSAMS documents are valid against the schema.

- The last development step would be to implement the query metrics that are used to estimate quickly if the node has the data for a particular query or not. See the *Query metrics support* section for the implementation details.

- Once the node plugin is tested and working, it may be deployed on the web server, as described in the *VAMDC-TAP node deployment* section. The node should be tested again with the VAMDC-TAP Validator working in the network mode.

CHAPTER

FOUR

NODE ARCHITECTURE

Java implementation of VAMDC-TAP node software is a web-service application implementing a RESTful interface according to VAMDC-TAP standard specification.

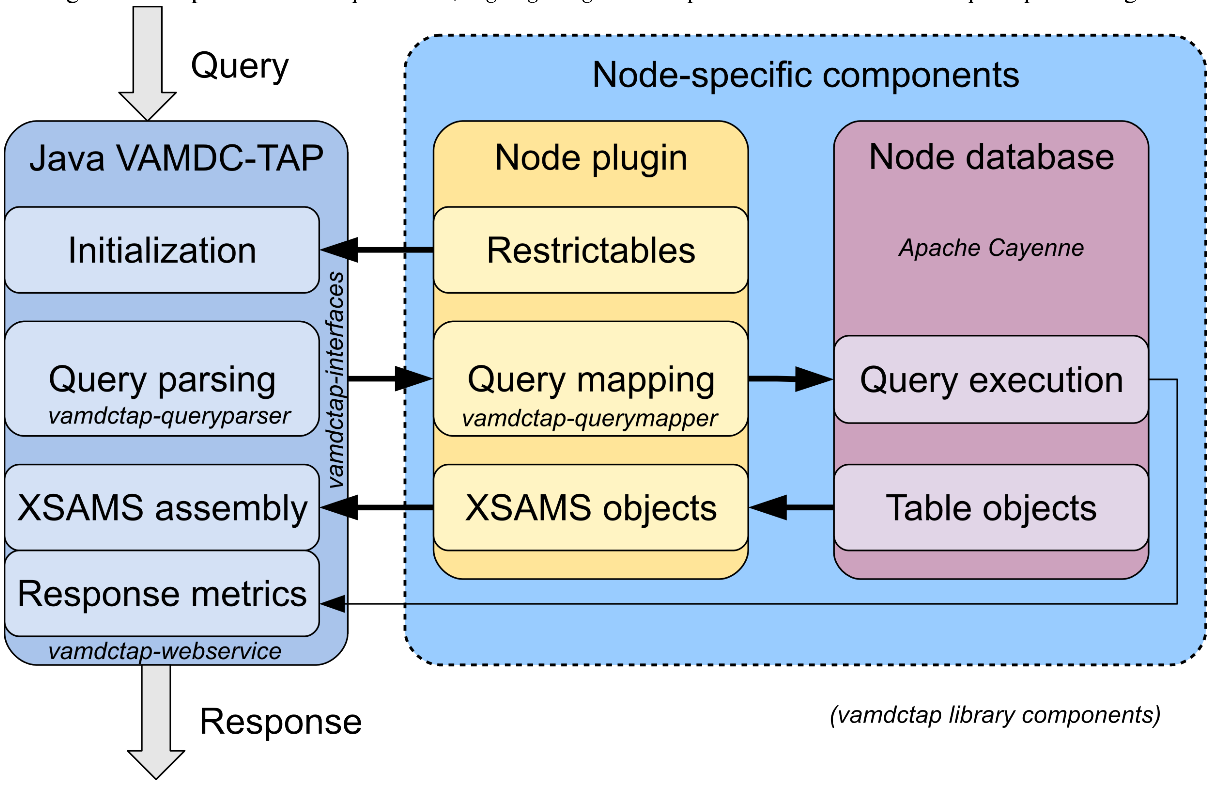
It is accessible using the HTTP protocol, with URLs like *http://node.name.tld/vamdc-tap/12_07/VOSI/capabilities* or *http://node.name.tld/vamdc-tap/12_07/TAP/sync?query=select%20species&lang=VSS2&format=XSAMS*. Here *http://node.name.tld/vamdc-tap/12_07/* is the node base url, **/VOSI/capabilities** and **/TAP/sync** are endpoint addresses, and *?query=select%20species&lang=VSS2&format=XSAMS* are HTTP request parameters.

For the complete list of endpoint addresses implemented please refer to section *Web-service endpoints*.

4.1 Request processing

During normal operation, node software receives *HTTP GET* and *HTTP HEAD* requests to the **/TAP/sync** endpoint. As a response to a request a valid XSAMS document and/or the HTTP response headers are sent.

The figure below presents the request flow, *highlighting* the components involved in the request processing.



During the request processing the few steps are performed. Java VAMDC-TAP implementation (**Framework**) handles the steps that are common for all VAMDC-TAP nodes. Node **Plugin** is responsible for the steps that are essentially node-specific. To access the **database**, the Apache Cayenne object-relational mapping framework is used.

- On the query reception, the **framework** asks the **plugin** for the list of supported **keywords** (Restrictables).
- The **Framework** parses the incoming query. The validity of the query is checked. A tree of objects is constructed, representing the logical structure of the query. For more details please refer to the *Query* section.
- **Framework** asks **Plugin** to construct the document by calling the *DatabasePlugin interface*

  buildXSAMS(RequestInterface incomingRequest) method. All the query information is accessible via the RequestInterface object passed as a parameter.
- **Plugin** maps the incoming query logical tree into one or more **Database** queries, as described in the *Query mapping scenarios* section.
- **Plugin** queries the **database** and retreives **Apache Cayenne** data objects. **XSAMS** elements are built from those data objects and are attached to the XSAMS document tree. See the *XSAMS tree building* section for the details.
- When the document tree is built, **Plugin** returns the control to the **Framework**.
- The **Framework** does the final checks on the document tree and calculates the accurate metrics for the document.
- The **Framework** converts the document tree into XML stream and sends it to the client.

4.2 Plugin and Framework Interfaces

Interaction between the database plugin and the Java node software is performed through two interfaces:

- **ref** *DatabasePlug*

  defined in the **org.vamdc.tapservice.api.DatabasePlugin** java interface and implemented by the node developer. Methods of this interface are called by the node software upon the arrival of a VAMDC-TAP request or during the initial startup and operation checks.
- **ref** *RequestInterface*

  defined in the **org.vamdc.tapservice.api.RequestInterface** java interface and implemented in the web-service framework. This interface is available to the node plugin to get the request information and feed the XSAMS blocks constructed.

4.2.1 DatabasePlugin interface

Each and every node plugin must implement the **org.vamdc.tapservice.api.DatabasePlugin** interface, defining the following methods:

- **public abstract Collection<Restrictable> getRestrictables();**

  Must return a collection of **org.vamdc.dictionary.Restrictable** dictionary keys that are supported by the node. This method is called once per each request to the */TAP/sync* and */VOSI/capabilities* endpoints.
- **public abstract void buildXSAMS (RequestInterface userRequest);**

  Build the XSAMS document tree corresponding to the incoming request. Object implementing *RequestInterface interface* is passed as a parameter. No return is expected. This method is called every time the node software is receiving an *HTTP GET* request to the */TAP/sync?* endpoint.

  WARNING! Node plugin class is instantiated only once when the node is started, all calls to buildXSAMS should be thread-safe to handle concurrent requests correctly.

  Implementation details are covered in the *XSAMS tree building* section.

- **public abstract Map<Dictionary.HeaderMetrics,Integer> getMetrics(RequestInterface userRequest);**

  Get the metrics corresponding to a query. This method is called for every incoming HEAD request to the */TAP/sync?* endpoint. *RequestInterface userRequest* parameter is identical to the one passed to buildXSAMS method. This method should return a map of VAMDC-COUNT-* HTTP header names and their estimate values. For header names and meaning, see the [VAMDC-TAP] documentation section DataAccessProtocol.

- **public abstract boolean isAvailable();**

  Do some really node-specific availability checks. This method is called periodically from the availability monitor. First call is initiated after the first request to the */VOSI/availability* service endpoint. Method may be used to temporary shutdown the node during the database maintenance, or to do some integrity checks on the database. Availability check interval may be set in the *Node Configuration File* option **self-check_interval**.

  WARNING! this method should not be used for doing periodic maintenance since it is never called before the first request to the */VOSI/availability* service endpoint.

4.2.2 RequestInterface interface

When the incoming request arrives to Java Node Software, methods of the *DatabasePlugin interface* are called, as described earlier. Methods of that interface accept as a parameter an object implementing the **org.vamdc.tapservice.api.RequestInterface**. That interface provides the access to the request information and the Java Node Software facilities.

Following methods are part of this interface:

- **public abstract boolean isValid();** this method returns **true** if the incoming request is valid and should be processed. If the returned value is **false**, the request should be considered as invalid, no processing is required.

  Query string may be obtained by calling the getQueryString method and saved by the node plugin for the logging purposes.

- **public abstract Query getQuery();** This method returns the base object of the QueryParser library, implementing the Query interface.

  That interface is described in detail in the *Query* section of this document.

- **public abstract LogicNode getQueryTree();**

  This is the shortcut method returning the root element of the logic tree corresponding to the incoming query.

- **public abstract Collection<RestrictExpression> getQueryKeywords();** This is an another shortcut method, allowing to get a collection of the keywords used in the incoming query. The keywords relation logic is omitted.

  WARNING! This method should not be used as the main source of data for the query mapping since it completely looses the query relation logic. Imagine the query:

  ```
  SELECT * WHERE AtomSymbol='Ca' OR AtomSymbol='Fe'
  ```

  If this method is used for the query mapping, this query would produce the same result as the query:

  ```
  SELECT * WHERE AtomSymbol='Ca' AND AtomSymbol='Fe'
  ```

  which is obviously incorrect.

- **public abstract String getQueryString();** The shortcut method to get the incoming query string.

- **public abstract boolean checkBranch(Requestable branch);** The shortcut method for the Query.checkBranch(), returns true if the result document is requested to contain a certain branch of XSAMS, specified by the **org.vamdc.dictionary.Requestable** name.

This method should be called in all builders to verify if a certain branch should be built, before even executing or mapping the queries.

The behaviour of the keywords is described in the VAMDC Dictionary documentation [VAMDCDict], the section **Requestables**

- **public abstract ObjectContext getCayenneContext();** Returns the Apache Cayenne object context. That is the main endpoint of the Cayenne ORM library. For more information on using the Apache Cayenne look in the sections *Database Object Model* and *Query mapping scenarios*.
- **public abstract XSAMSManager getXsamsManager();** Get an instance of the XSAMS document manager. This manager contains several helper methods for building the XSAMS document. All XSAMS branches built by the node plugin should be attached to it. Check the *XSAMS tree building* section for more details.
- **public abstract void setLastModified(Date date);**

  Sets the last-modified header of the response. This method may be called several times during the request processing. If called more than once, the last modification date is updated only if the subsequent date is newer than the value communicated before.

CHAPTER

FIVE

DATABASE PLUGIN TESTING

To test the node plugin, the VAMDC-TAP Validator software may be used. It implements the same DatabasePlugin interface call logic and RequestInterface methods operation as the VAMDC-TAP node webservice. All the dependency libraries are bundled in a single TAPValidator.jar archive.

Such an approach facilitates the node plugin development: there is no need to install the application server and deploy web service framework on the development machine.

To use the TAPValidator for the plugin development, few steps are required:

- The most recent version of TAPValidator.jar should be added to the project library path.
- New Java Application run/execution configuration should be defined, indicating the **org.vamdc.validator.ValidatorMain** as the main class.
- TAPValidator should be configured to operate in the plugin development mode. In the Settings window, plugin mode radiobutton should be selected; The class name implementing the *DatabasePlugin interface* should be indicated, including the java package name.

If everything is set up correctly, the list of supported restrictables should appear in the right-top text area. Plugin **buildXSAMS(...)** method is called every time the *Query* button is pressed.

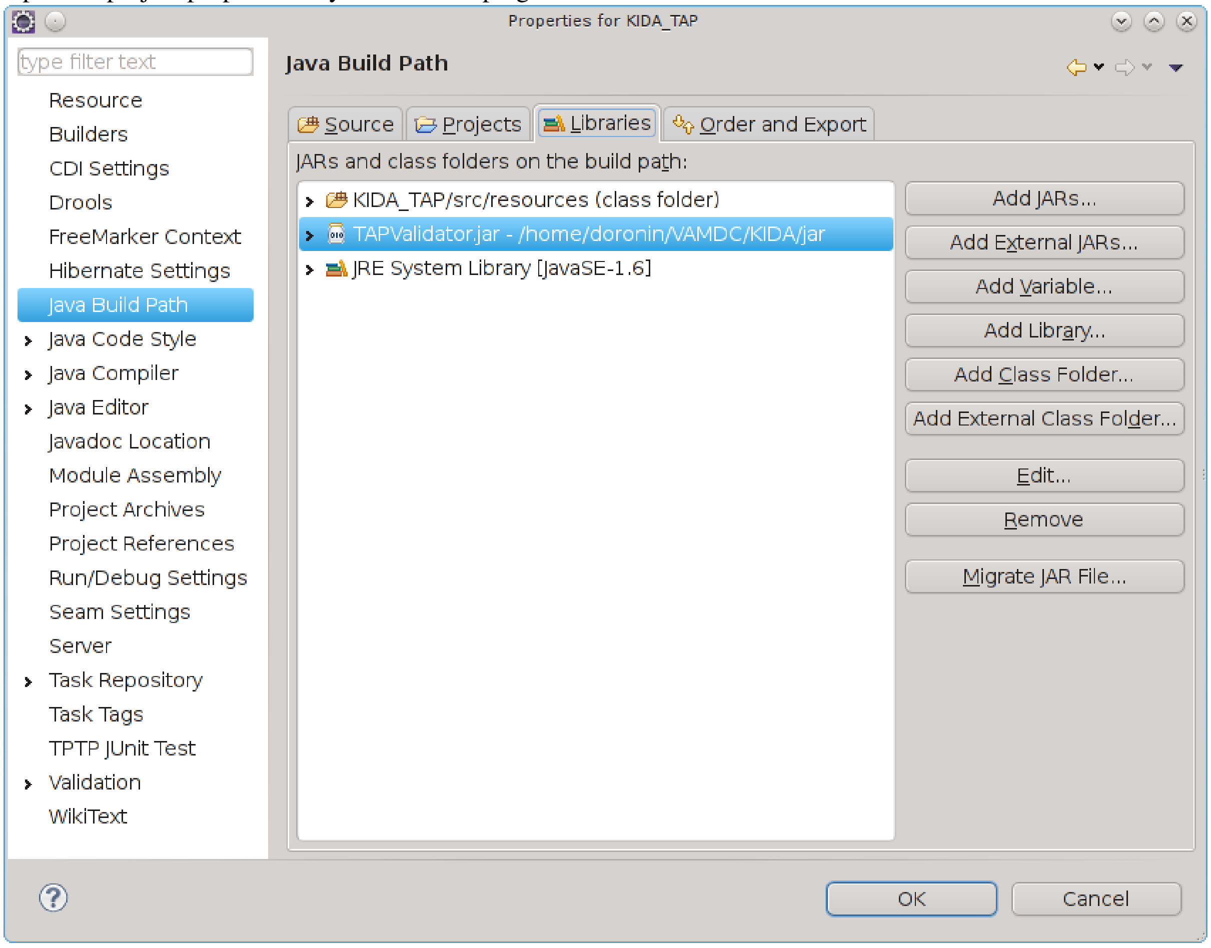
For more information on the VAMDC-TAP Validator user interface and features, please refer to the [TAPValidator] documentation.

5.1 Eclipse project setup / Screenshots

The screenshots corresponding to the Eclipse project setup are presented below.

5.1.1 Adding VAMDC-TAP Validator to the build path

Open the project properties of your database plugin.

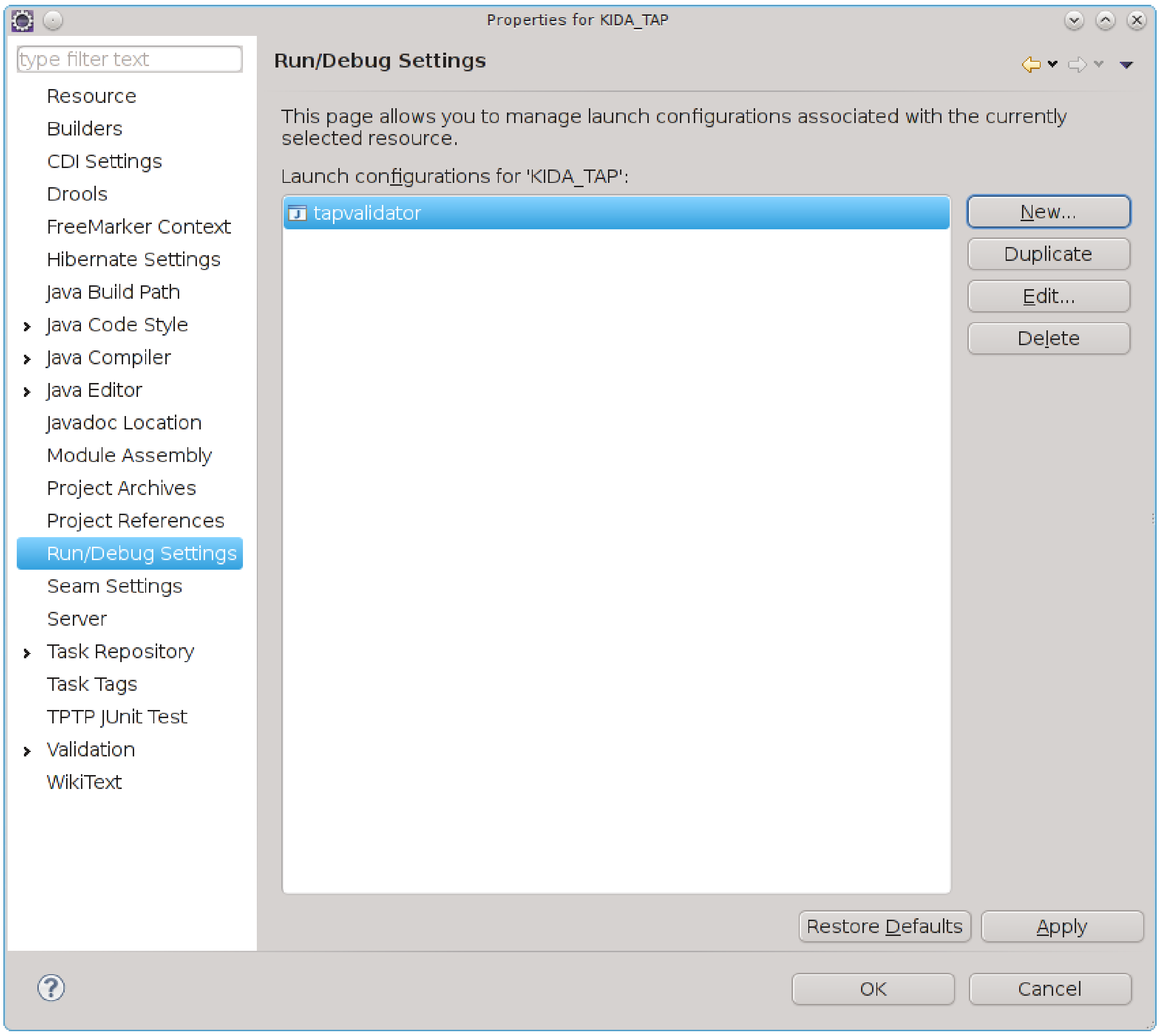


JARs and class folders on the build path:

- KIDA_TAP/src/resources (class folder)
- TAPValidator.jar - /home/doronin/VAMDC/KIDA/jar
- JRE System Library [JavaSE-1.6]

Add the latest VAMDC-TAP Validator JAR to the build path by clicking on the “Add external JARs” button

5.1.2 Managing run configurations


Properties for KIDA_TAP

type filter text

Resource
Builders
CDI Settings
Drools
FreeMarker Context
Hibernate Settings
Java Build Path
Java Code Style
Java Compiler
Java Editor
Javadoc Location
Module Assembly
Project Archives
Project References
Run/Debug Settings
Seam Settings
Server
Task Repository
Task Tags
TPTP JUnit Test
Validation
WikiText

Run/Debug Settings

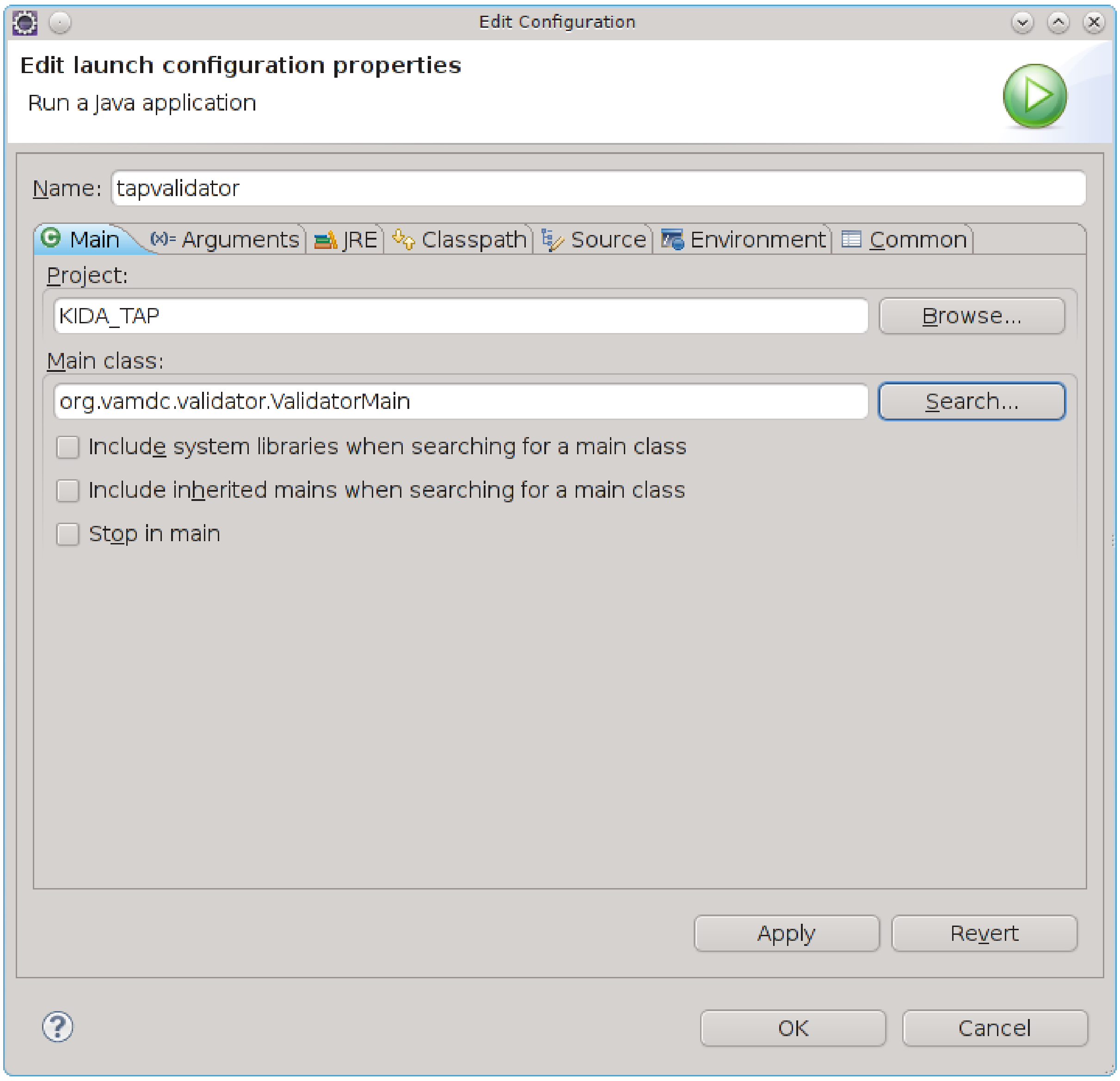
This page allows you to manage launch configurations associated with the currently selected resource.

Launch configurations for 'KIDA_TAP':

tapvalidator

Setup a new run configuration by clicking the “New...” button

5.1.3 Creating run configuration


Edit Configuration

Edit launch configuration properties

Run a Java application

Name: tapvalidator

Project: KIDA_TAP

Main class: org.vamdc.validator.ValidatorMain

☐ Include system libraries when searching for a main class

☐ Include inherited mains when searching for a main class

☐ Stop in main

Create a new run configuration with the **org.vamdc.validator.ValidatorMain** Main class path

5.2 Maven Integration

All Java software developed as a part of VAMDC is available at VAMDC Maven repository

http://nexus.vamdc.org/nexus/content/repositories/releases/

To use Maven for dependency management of your plugin, a following sample POM.xml may be used:

```
<project xmlns="http://maven.apache.org/POM/4.0.0"
        xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
        xsi:schemaLocation="http://maven.apache.org/POM/4.0.0
                http://maven.apache.org/xsd/maven-4.0.0.xsd">
        <modelVersion>4.0.0</modelVersion>
        <groupId>org.vamdc.%databasename%</groupId>
        <artifactId>plugin</artifactId>
        <name>databasename plugin for java node software</name>

        <repositories>
                <repository>
                        <id>nexus</id>
                        <name>VAMDC Releases</name>
                        <url>http://nexus.vamdc.org/nexus/content/groups/public/</url>
                </repository>
        </repositories>

        <parent>
                <groupId>org.vamdc.tap</groupId>
                <artifactId>vamdctap-plugin</artifactId>
                <version>12.07r2</version>
        </parent>

        <dependencies>
                <dependency>
                        <groupId>org.vamdc.%databasename%</groupId>
                        <artifactId>database_dao</artifactId>
                        <version>0.0.1-SNAPSHOT</version>
                </dependency>
                <dependency>
                        <groupId>org.vamdc</groupId>
                        <artifactId>TAPValidator</artifactId>
                        <version>12.07r2</version>
                        <type>jar</type>
                        <scope>compile</scope>
                </dependency>
        </dependencies>
</project>
```

All the required dependencies are included in the *parent* project, **vamdctap-plugin**

CHAPTER

SIX

DATABASE OBJECT MODEL

Java VAMDC-TAP node software implementation suggests and supports the use of Apache Cayenne Object-Relational Mapping (ORM) library.

Apache Cayenne supports various database engines, such as MySQL, PostgreSQL, SQLite, Oracle, DB2, Microsoft SQL Server.

Creation of database objects is made simple thanks to the graphical modeler application, provided as a part of Cayenne.

Process of creating and using a database model is well described in the project official documentation [CAYDOC] and there is no need to repeat it in this document. Reading the Cayenne documentation is a **MUST** for the understanding and creating efficient query mapper routines and high performance database access classes.

6.1 Step-by-step guide

Here is a small illustrated guide on creating database mappings. We will need Cayenne modeler application, it can be downloaded from http://cayenne.apache.org/download.html as a part of binary distribution.

Version 3.1 is recommended for use with the 12.07r2 version of the Java VAMDC-TAP Node Software.

6.1.1 Create maven project

First we need to generate a Maven project:

```
mvn archetype:generate \
  -DarchetypeGroupId=org.apache.maven.archetypes \
  -DgroupId=org.vamdc.database \
  -DartifactId=daoclasses
```

and create folder src/main/resources where we will put cayenne modeler files.

Maven pom.xml can be replaced with the following contents:

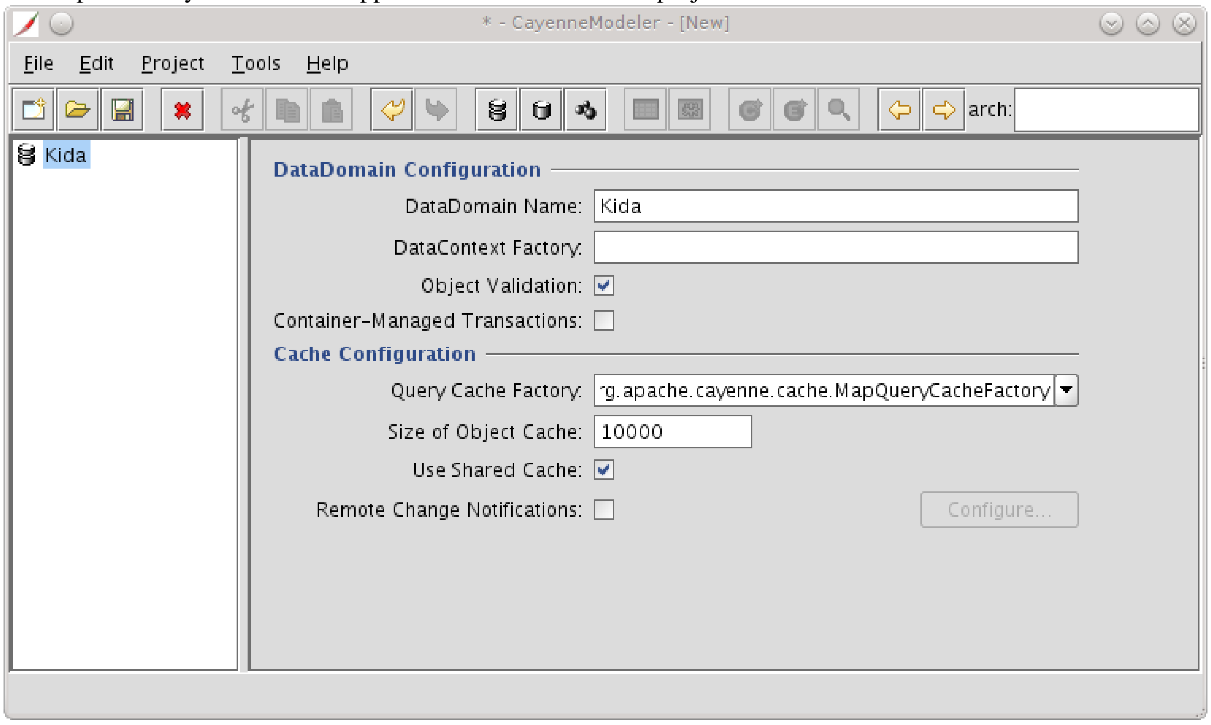
```
<project xmlns="http://maven.apache.org/POM/4.0.0"
        xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
        xsi:schemaLocation="http://maven.apache.org/POM/4.0.0
                http://maven.apache.org/xsd/maven-4.0.0.xsd">
        <modelVersion>4.0.0</modelVersion>
        <groupId>org.vamdc.databaseName</groupId>
        <artifactId>node_dao</artifactId>
        <version>12.07r2</version>
        <name>databaseName database objects</name>

        <parent>
                <groupId>org.vamdc.tap</groupId>
                <artifactId>cayenne_dao</artifactId>
                <version>12.07r2</version>
        </parent>

        <repositories>
                <repository>
                        <id>vamdc repository</id>
                        <name>VAMDC stuff for Maven</name>
                        <url>http://nexus.vamdc.org/nexus/content/repositories/releases</url>
                        <layout>default</layout>
                </repository>
        </repositories>
</project>
```

6.1.2 Create Cayenne classes

Let's open the cayenne modeler application and create a new project:



DataDomain Configuration

DataDomain Name: Kida

DataContext Factory:

Object Validation: ✓

Container-Managed Transactions: ☐

Cache Configuration

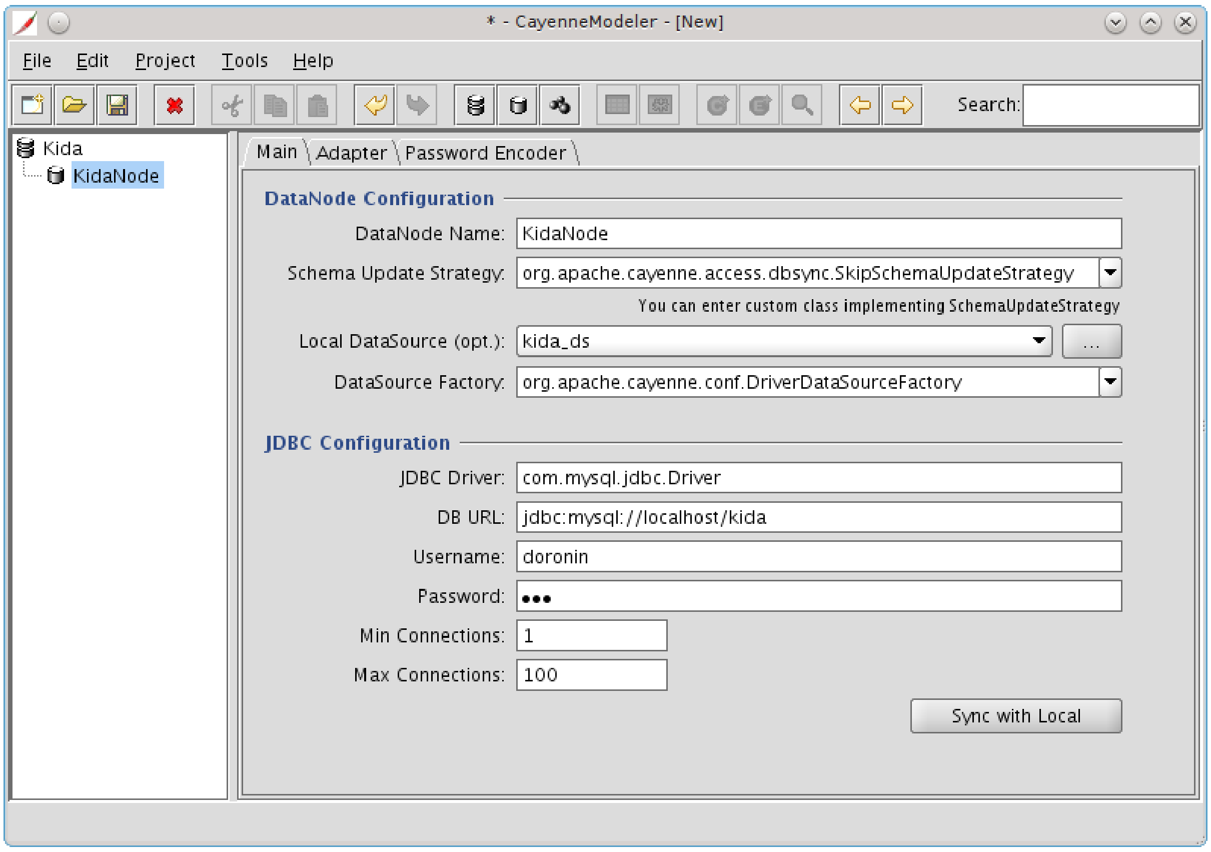
Query Cache Factory: ·g.apache.cayenne.cache.MapQueryCacheFactory

Size of Object Cache: 10000

Use Shared Cache: ✓

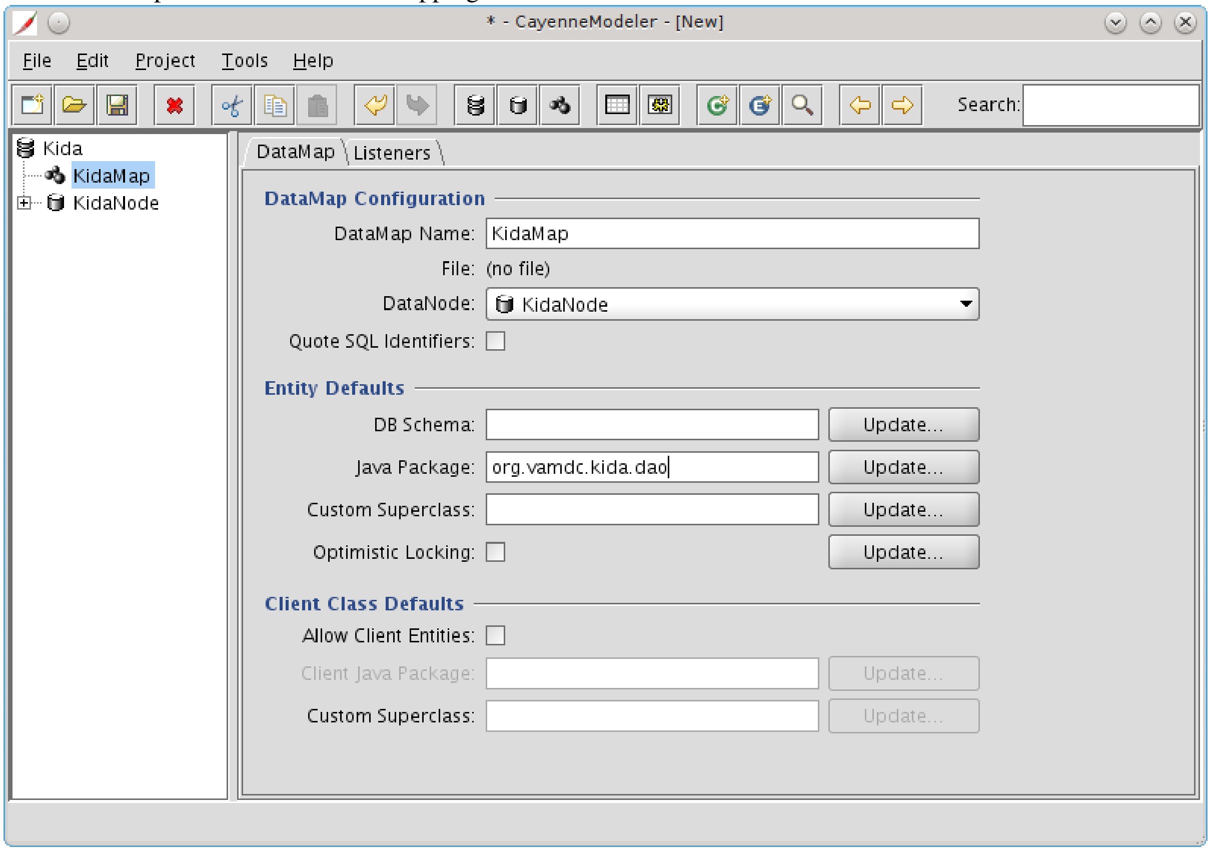
Remote Change Notifications: ☐

Now we need a dataNode describing the database connection


* - CayenneModeler - [New]
File Edit Project Tools Help
Search:
Kida
KidaNode
Main Adapter Password Encoder
DataNode Configuration
JDBC Configuration
...
Sync with Local

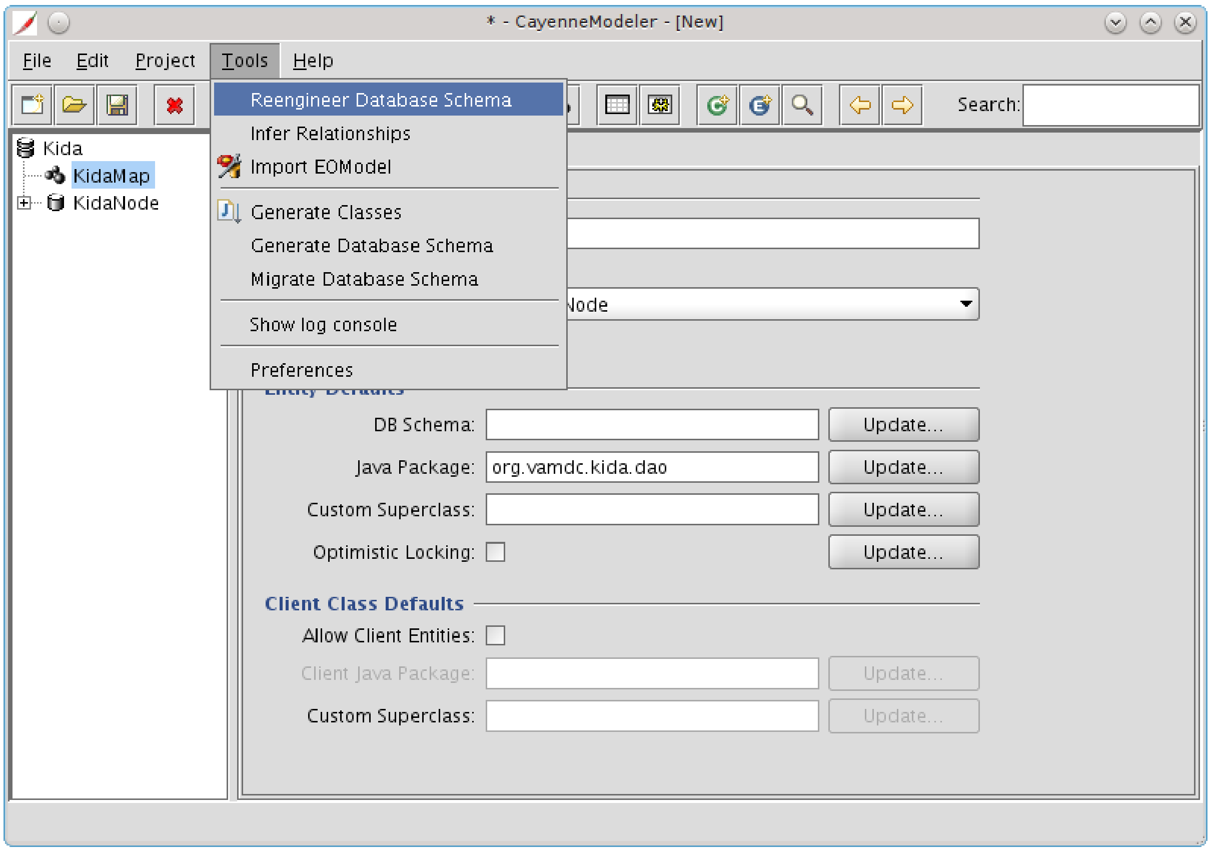
DataNode Name: KidaNode
Schema Update Strategy: org.apache.cayenne.access.dbsync.SkipSchemaUpdateStrategy
You can enter custom class implementing SchemaUpdateStrategy
Local DataSource (opt.): kida_ds
DataSource Factory: org.apache.cayenne.conf.DriverDataSourceFactory
JDBC Driver: com.mysql.jdbc.Driver
DB URL: jdbc:mysql://localhost/kida
Username: doronin
Password: •••
Min Connections: 1
Max Connections: 100

And a dataMap that will contain all mapping tables and classes



DataMap Name: KidaMap
File: (no file)
DataNode: KidaNode
Quote SQL Identifiers: ☐
DB Schema:
Java Package: org.vamdc.kida.dao
Custom Superclass:
Optimistic Locking: ☐
Allow Client Entities: ☐
Client Java Package:
Custom Superclass:

After the DataMap is created, we need to import the database schema:



DB Schema:

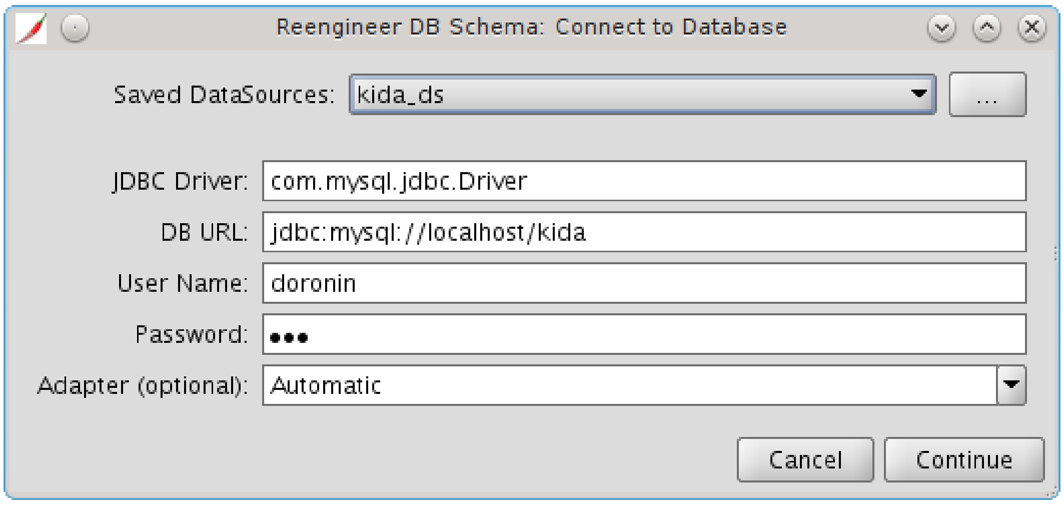
Java Package: org.vamdc.kida.dao

Custom Superclass:

Optimistic Locking: ☐

Allow Client Entities: ☐

Custom Superclass:


Reengineer DB Schema: Connect to Database

Saved DataSources: kida_ds

JDBC Driver: com.mysql.jdbc.Driver

DB URL: jdbc:mysql://localhost/kida

User Name: doronin

Password: ●●●

Adapter (optional): Automatic

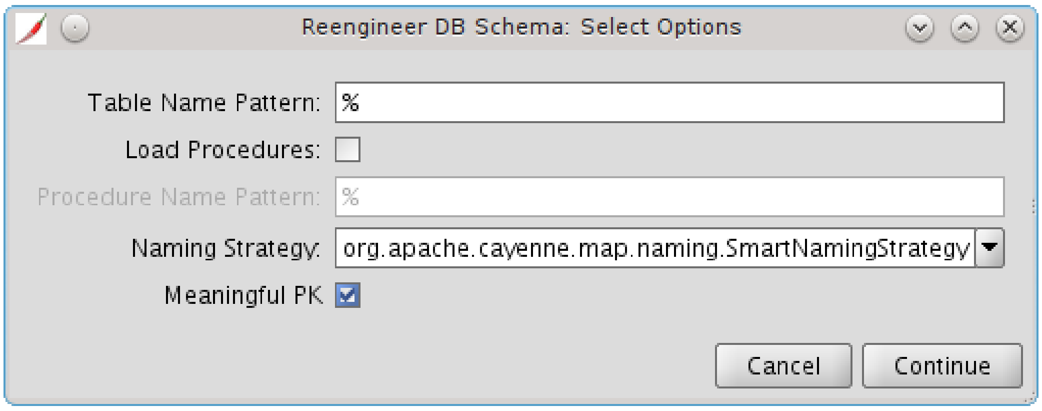

Reengineer DB Schema: Select Options

Table Name Pattern: %

Load Procedures: ☐

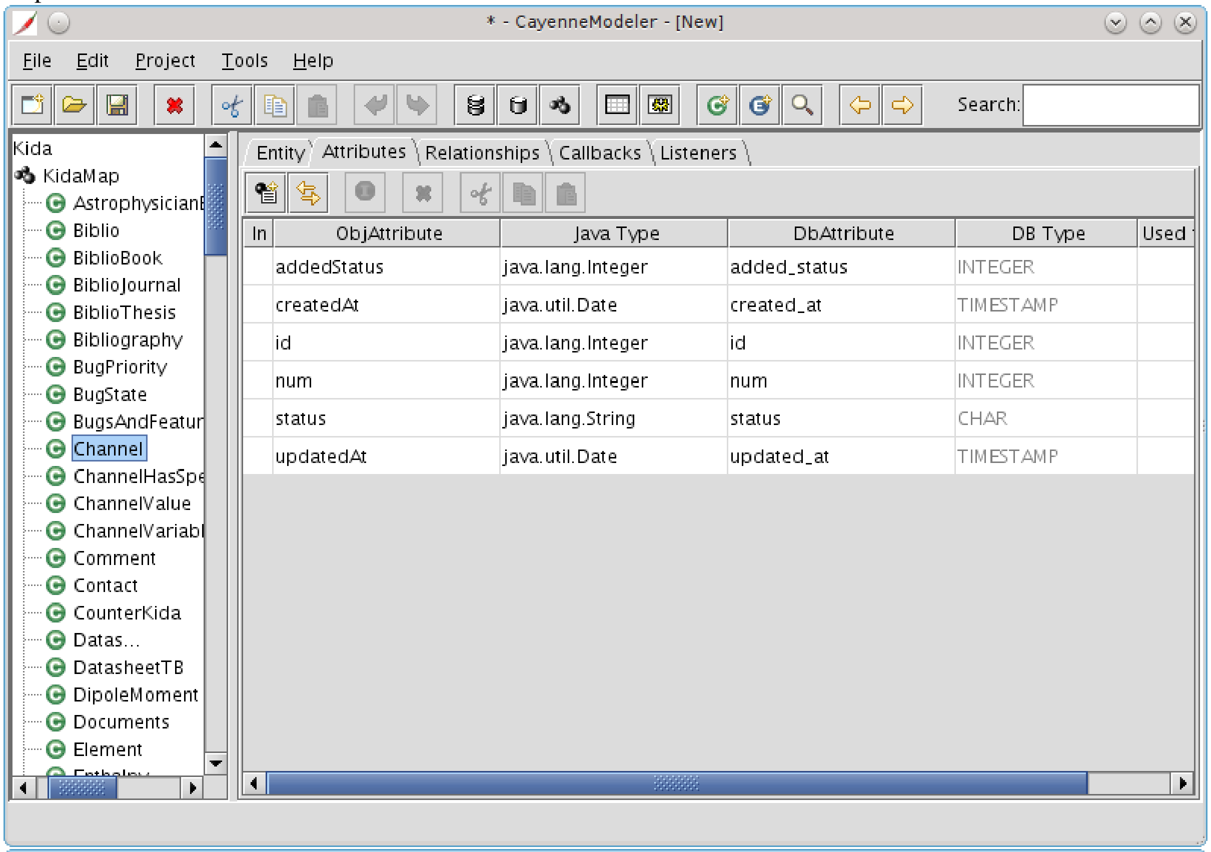
Procedure Name Pattern: %

Naming Strategy: org.apache.cayenne.map.naming.SmartNamingStrategy

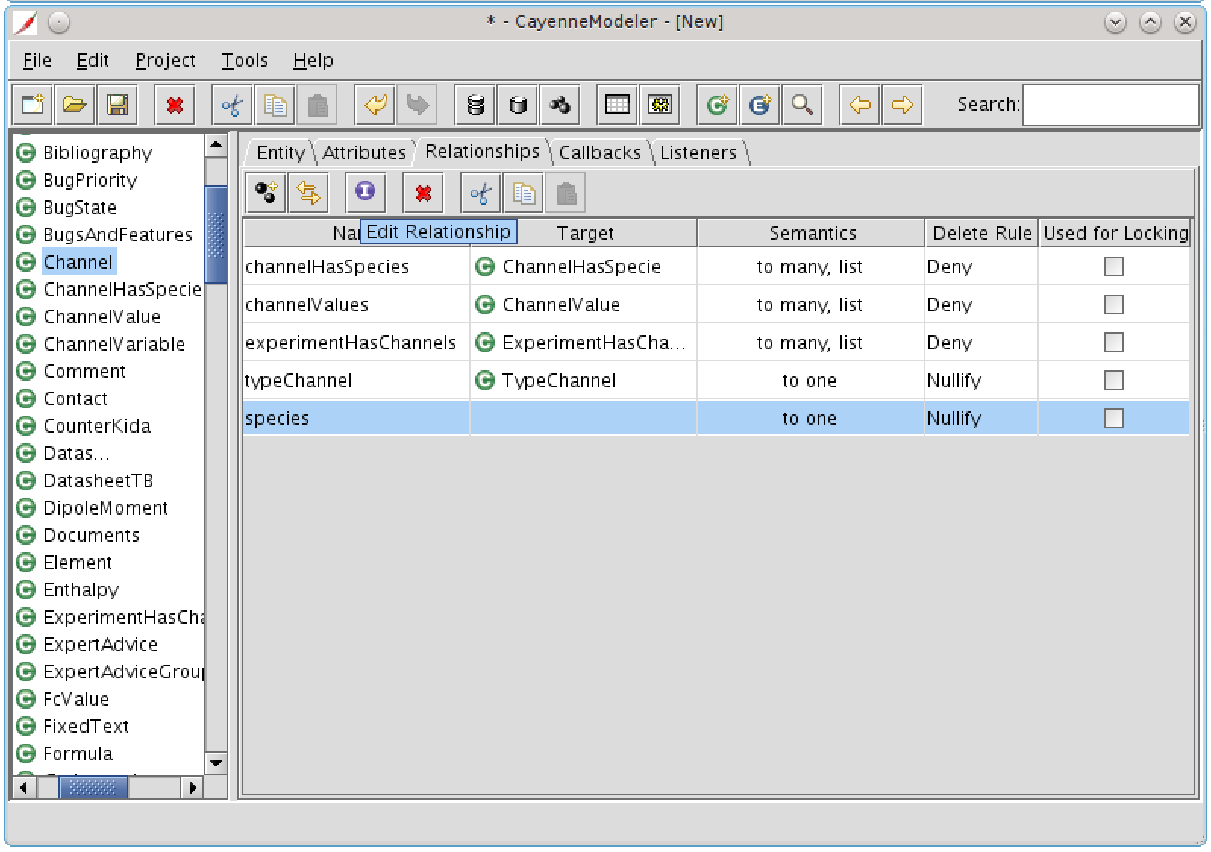
Meaningful PK ✓

!Note the “Meaningful PK” flag is set to preserve the getter methods for the primary key fields.

As a result a separate Java class is generated for each database table table, containing attribute fields and relationship references.

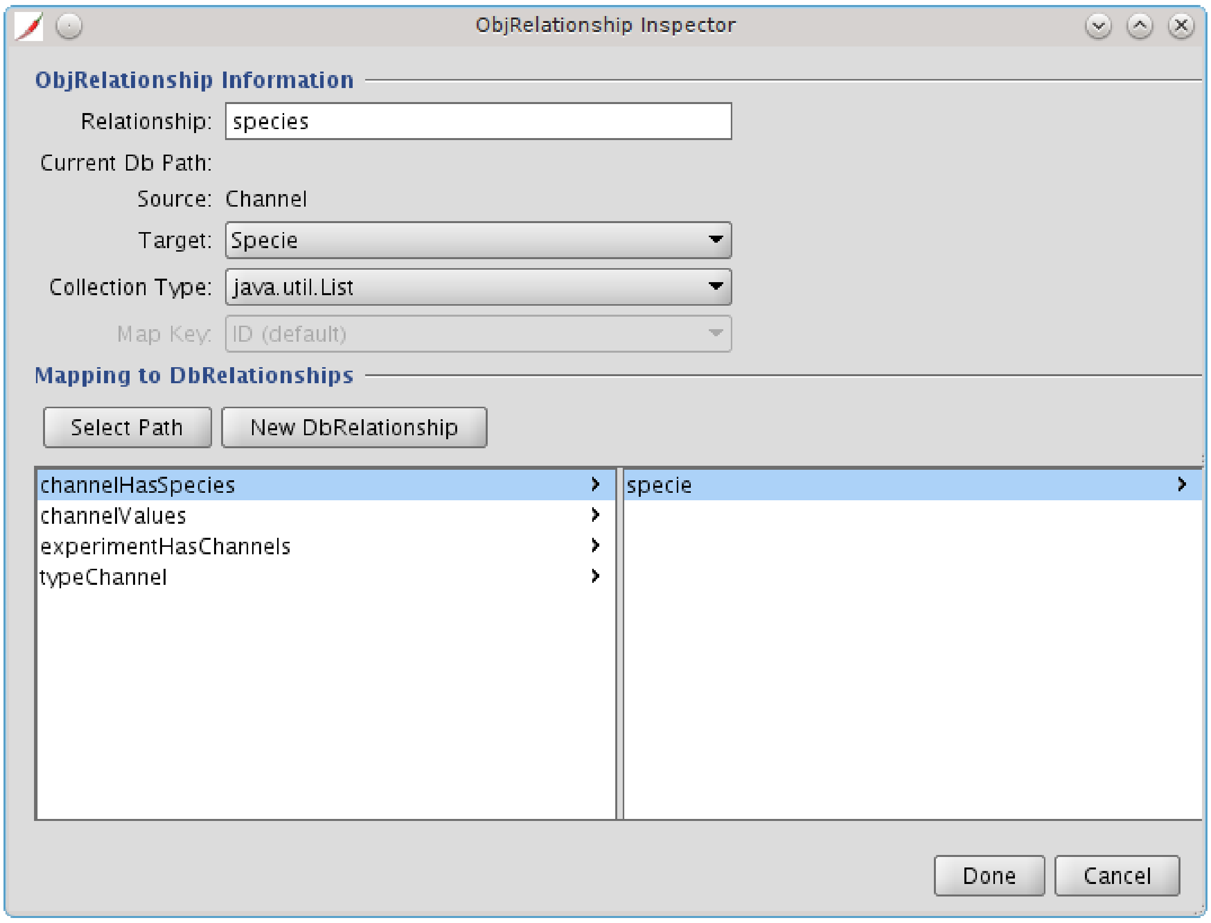


In	ObjAttribute	Java Type	DbAttribute	DB Type	Used
	addedStatus	java.lang.Integer	added_status	INTEGER	
	createdAt	java.util.Date	created_at	TIMESTAMP	
	id	java.lang.Integer	id	INTEGER	
	num	java.lang.Integer	num	INTEGER	
	status	java.lang.String	status	CHAR	
	updatedAt	java.util.Date	updated_at	TIMESTAMP	

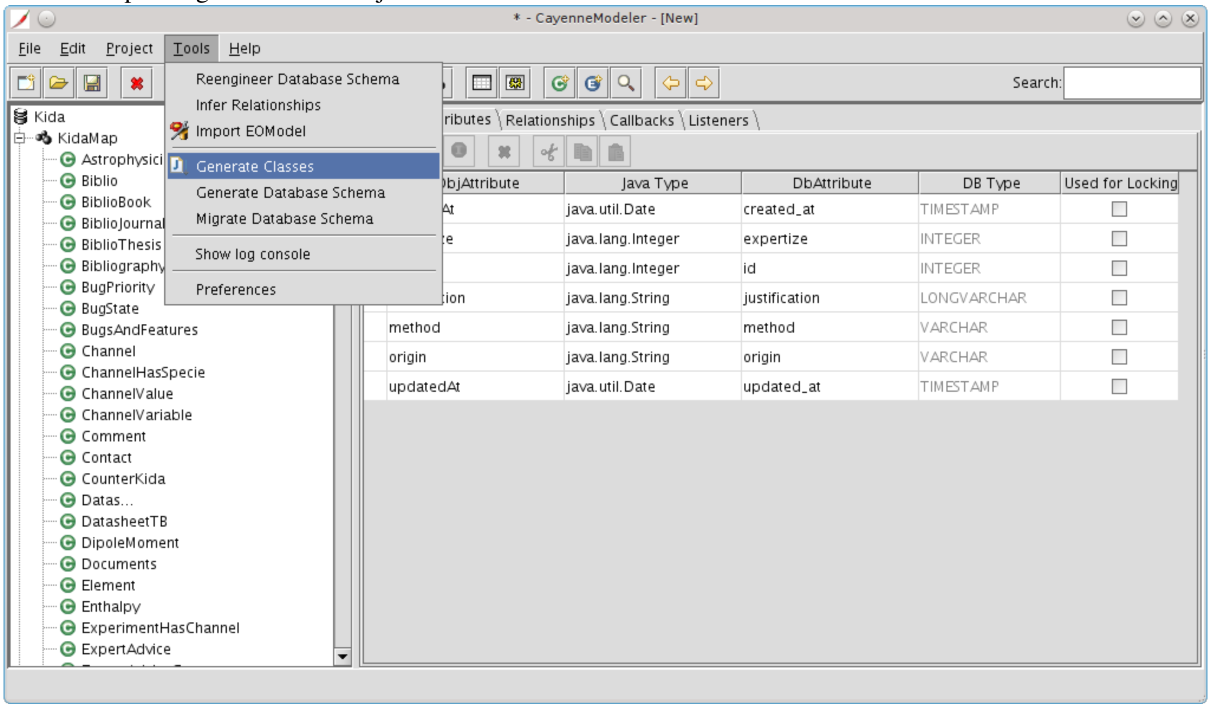


Na	Target	Semantics	Delete Rule	Used for Locking
channelHasSpecies	ChannelHasSpecie	to many, list	Deny	☐
channelValues	ChannelValue	to many, list	Deny	☐
experimentHasChannels	ExperimentHasCha...	to many, list	Deny	☐
typeChannel	TypeChannel	to one	Nullify	☐
species		to one	Nullify	☐

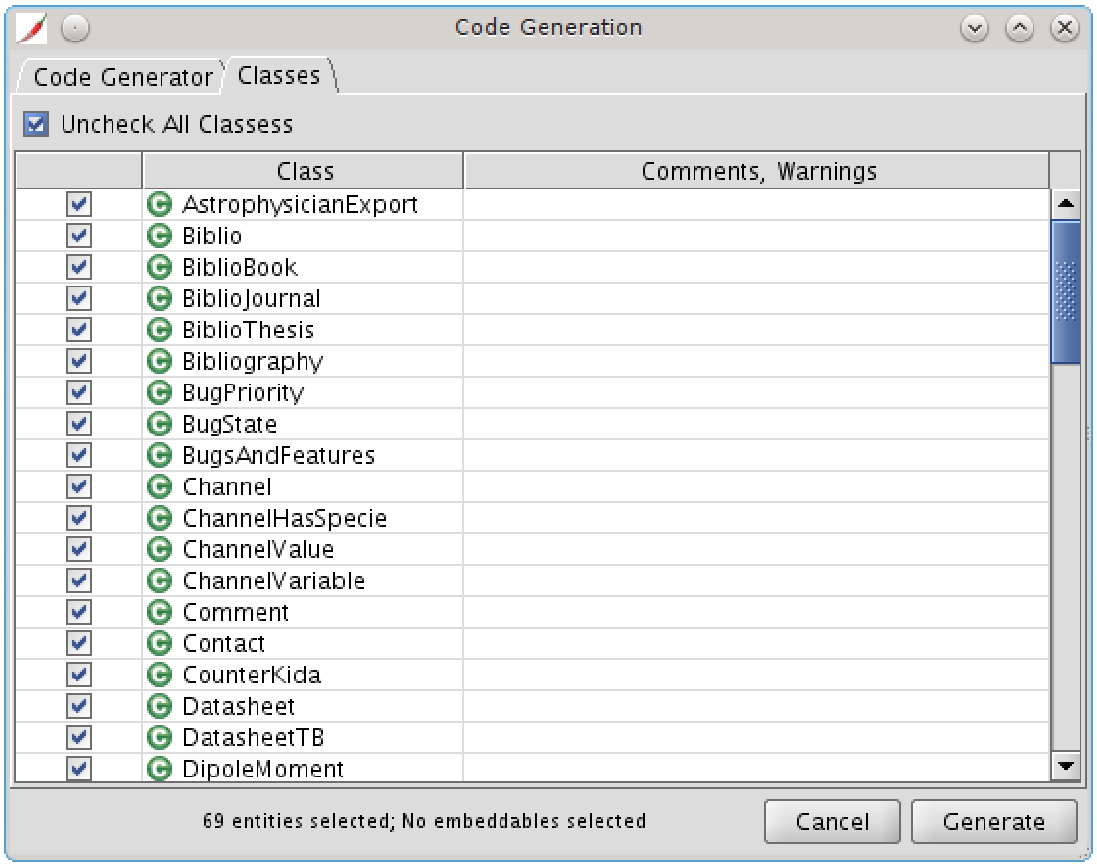
For many-to-many relations relationships need to be created manually: create a new relationship, press on the violet I button, indicate the path in the bottom of the window.



The last step is to generate class objects:



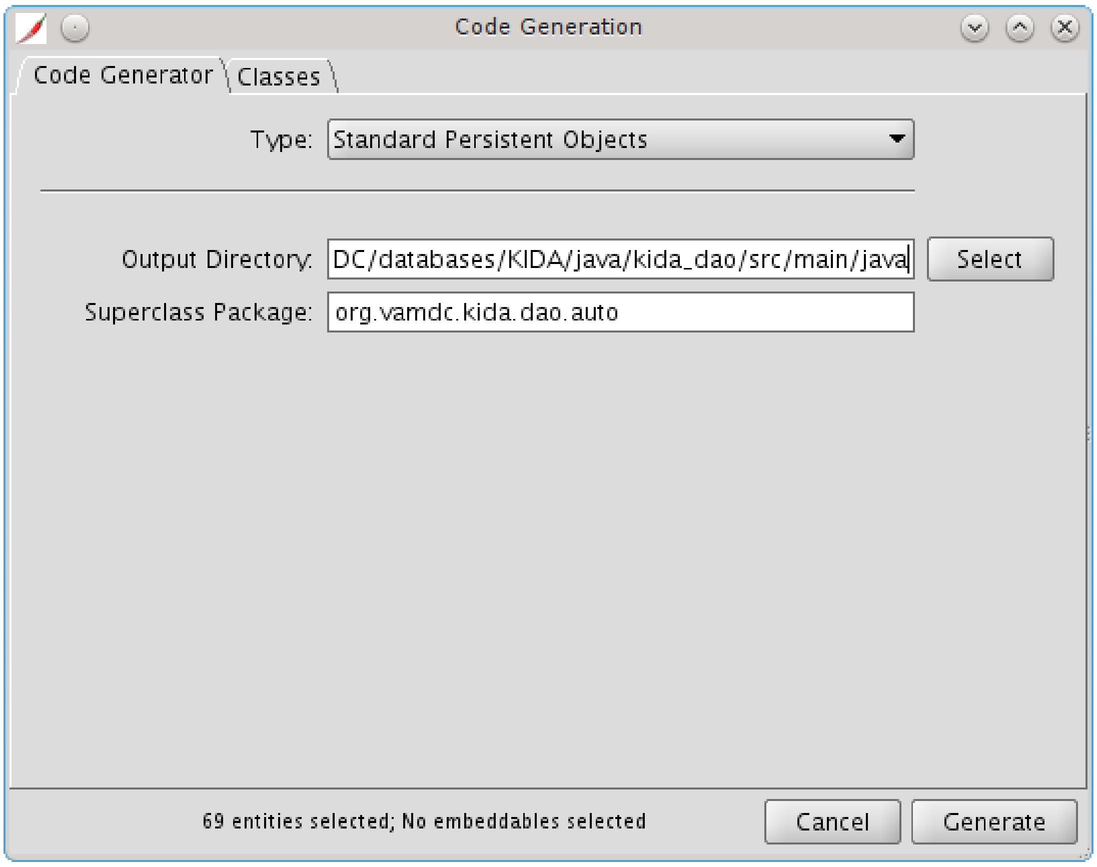
ObjAttribute	Java Type	DbAttribute	DB Type	Used for Locking
At	java.util.Date	created_at	TIMESTAMP	☐
e	java.lang.Integer	expertize	INTEGER	☐
	java.lang.Integer	id	INTEGER	☐
ion	java.lang.String	justification	LONGVARCHAR	☐
method	java.lang.String	method	VARCHAR	☐
origin	java.lang.String	origin	VARCHAR	☐
updatedAt	java.util.Date	updated_at	TIMESTAMP	☐



☑ Uncheck All Classess

	Class	Comments, Warnings
☑	AstrophysicianExport	
☑	Biblio	
☑	BiblioBook	
☑	BiblioJournal	
☑	BiblioThesis	
☑	Bibliography	
☑	BugPriority	
☑	BugState	
☑	BugsAndFeatures	
☑	Channel	
☑	ChannelHasSpecie	
☑	ChannelValue	
☑	ChannelVariable	
☑	Comment	
☑	Contact	
☑	CounterKida	
☑	Datasheet	
☑	DatasheetTB	
☑	DipoleMoment	

69 entities selected; No embeddables selected



Type: Standard Persistent Objects

Output Directory: DC/databases/KIDA/java/kida_dao/src/main/java

Superclass Package: org.vamdc.kida.dao.auto

69 entities selected; No embeddables selected

As a destination directory, src/main/java of Maven project needs to be specified. Cayenne project itself needs to be saved next to it, in src/main/resources.

6.2 Notable Cayenne features used

The use of an ORM framework provides several benefits:

- Object-oriented view of the database;
- Automatic relations traversal using the object methods (explained below);
- Simplified translation of the incoming queries (see *VSS query parsing and mapping*)

6.2.1 Relations traversing

If properly defined, database model contains information about all table relations by means of the foreign keys. While constructing the query, those relations can be automatically traversed to form the correct query with desired selection criterias.

As an example, let us have a look at the case of two tables, **'artists'** and **'albums'**, with a one-to-one mapping of albums to artists using the foreign key **'albumArtist'** pointing to the **'id'** field of the **'artists'** table.

artists	
id	**name**
1	Elton John
2	Michael Jackson
3	Joe Cocker

and

albums			
id	**artistId**	**name**	**year**
1	1	The Big Picture	1997
2	1	Goodbye Yellow Brick Road	1973
3	2	Off the Wall	1979
4	2	Invincible	2001
5	3	Across from Midnight	1997
6	3	Respect Yourself	2002

For the table **'albums'** we have one-to-one relation with the **'artists'** table, called **'albumArtist'** and for artists the reverse one-to-many relationship **'artistAlbums'**

So, if we want to get all artists that released albums in 1997, we would create an **Expression** containing the path from the **'artists'** table to the **'year'** field of **'albums'** table and the expression type **'match'**

```
Expression exp = ExpressionFactory.matchExp("artistAlbums.year", 1997);
SelectQuery query = new SelectQuery(Artists.class,exp);
List<Artists> artists = context.performQuery(query);
```

To add another constraint on a query, we may redefine the Expression:

```
exp = exp.andExp(ExpressionFactory.likeExp("name", "%Cocker%"));
```

Once we received the artists list, we may get the name of each artist, or have a look at all his albums:

```
for (Artists artist:artists){
  System.out.println("name: "+artist.Name+":");
  for (Albums album:artist.getArtistAlbums()){
    System.out.println("    Album: "+album.Name+"("+album.Year+")");
  }
}
```

This code should print something like:

```
Elton John:
    Album: The Big Picture(1997)
    Album: Goodbye Yellow Brick Road(1973)
```

```
Joe Cocker:
    Album: Across from Midnight(1997)
    Album: Respect Yourself(2002)
```

For the case of VAMDC node plugin, none of the expressions would require 'manual' construction: they will be translated from the incoming queries. Query translation is described in a separate chapter *Query mapping scenarios*

6.2.2 Path aliases

Imagine that we have the scenario of many-to-many relation through a separate table. For the previous example, let's add a table **'albumartist'** with three columns, **'id'**, **'artistId'** and **'albumId'** Table **'albums'** does not contain the 'artistID' column any more, but both forward and reverse relations are still called **'albumArtists'** and **'artistAlbums'**

Let us imagine that we need to select the artists that released their albums both in 1973 and 1997.

Joining expressions neither with exp.andExp nor exp.orExp would give us appropriate queries.

exp.andExp() would produce a query:

```
SELECT DISTINCT t0.name, t0.id
  FROM artist t0
  JOIN albumartist t1 ON (t0.id = t1.idArtist)
  JOIN album t2 ON (t1.idAlbum = t2.id)
  WHERE (t2.year = 1973) AND (t2.year = 1997)
```

that obviously never returns the data since the WHERE sub-conditions are mutually exclusive.

exp.orExp() would produce a query:

```
SELECT DISTINCT t0.name, t0.id
  FROM artist t0
  JOIN albumartist t1 ON (t0.id = t1.idArtist)
  JOIN album t2 ON (t1.idAlbum = t2.id)
  WHERE (t2.year = 1973) OR (t2.year = 1997)
```

that returns all the artists that released albums either in 1973 or 1997.

To resolve the problem, Apache Cayenne provides the aliases mechanism:

```
Expression e1 = ExpressionFactory.match("artistAlbumsAlias1.year", 1997);
Expression e2 = ExpressionFactory.match("artistAlbumsAlias2.year", 1973);
Expression e = e1.andExp(e2);
SelectQuery q = new SelectQuery(Artists.class, e);
q.aliasPathSplits("artistAlbums", "artistAlbumsAlias1", "artistAlbumsAlias2");
```

That last command tells the select query how to interpret the alias. Because the aliases are different, the SQL generated will have two completely separate set of joins:

```
SELECT DISTINCT t0.name, t0.id
  FROM artist t0
  JOIN albumartist t1 ON (t0.id = t1.idArtist)
  JOIN album t2 ON (t1.idAlbum = t2.id)
  JOIN albumartist t3 ON (t0.id = t3.idArtist)
  JOIN album t4 ON (t3.idAlbum = t4.id)
  WHERE (t2.year = 1997) AND (t4.year = 1973)
```

This is called "split path" in the Apache Cayenne terms.

If applied to the case of VAMDC databases, this approach may be used for handling the cases where the data is linked through a separate join table, such as articles by author or year, or reactants in chemical reaction databases.

CHAPTER

SEVEN

XSAMS TREE BUILDING

XSAMS is an XML schema, adopted within VAMDC for data exchange.

Java node software implementation uses JAXB library to establish the mapping between Java objects and XML elements and to read/write XSAMS documents

Each node plugin is responsible for building object trees corresponding to the XSAMS document branches and for attaching them to the main tree, managed by the node software. Once the node plugin has finished building the XSAMS document and returned from the buildXSAMS() method, the node software outputs the XML document to the client.

Java objects corresponding to every element of XSAMS schema are generated using JAXB library and are a part of *org.vamdc.xsams* package, included in **xsams** and **xsams-extra** libraries.

XSAMS objects can be constructed by extension of Jaxb mapping classes with convenience methods, provided within **xsams-extra** library. Constructors can receive Cayenne mapping objects as argument and initialize appropriate mapping XML fields. Such an approach allows to instantly apply an arbitrary processing to any field/element value or their combinations.

7.1 Example constructor class

As an example let's look at the BASECOL Source element constructor:

```
package org.vamdc.basecol.xsams;

import org.vamdc.basecol.dao.RefsArticles;
import org.vamdc.basecol.dao.RefsGroups;
import org.vamdc.xsams.XSAMSManager;
import org.vamdc.xsams.schema.SourceCategoryType;
import org.vamdc.xsams.schema.SourceType;
import org.vamdc.xsams.util.IDs;

public class Source extends SourceType{

        public Source(RefsArticles article){

                setSourceID(IDs.getSourceID(article.getArticleID().intValue()));
                setCategory(SourceCategoryType.fromValue(article.getJournalRel().getCategory()));

                setSourceName(article.getJournalRel().getSmallName());

                //Year
                setYear(article.getYear().intValue());

                //Authors
                setAuthors(new Authors(article.getFlatAuthorRel()));
                //Title
                setTitle(article.getTitle());
                //URL
                setUniformResourceIdentifier(article.getUrl());
                //Volume
                setVolume(article.getVolume());
                //Pages
                String pagesbe = article.getPage();
                if (pagesbe!=null){

                        if (pagesbe.contains("-")){
                                fillPages(pagesbe,"-");
                        }else if (pagesbe.contains("\\+")){
                                fillPages(pagesbe,"+");
                        }
                };

        }
}
```

The full source is available in **org.vamdc.basecol.xsams.Source** class.

Here, RefsArticles is the BASECOL Cayenne mapping object identifying one source record in the database, and SourceType is a root element of XSAMS Sources branch. SourceType is defined by the class **org.vamdc.xsams.schema.SourceType**.

Collection of RefsArticles objects is retrieved automatically through the Cayenne model relation. For each *Source* element we need to check if it is already attached to the XSAMS Document tree. If no existent object is found, the aforementioned builder is called and the generated object is attached to the document tree.:

```
public static List<SourceType> getSources(
                List<RefsGroups> referenceRel,
                XSAMSManager document,
                boolean filterSource) {

        ArrayList<SourceType> result = new ArrayList<SourceType>();

        /*always add the database self-reference*/
        result.add(document.getSource(IDs.getSourceID(0)));

        if (referenceRel==null) return result;

        /*Add all sources that are stated as 'isSource'*/
        for (RefsGroups myref:referenceRel){
                RefsArticles article = myref.getArticleRel();
                if (article!=null && (myref.getIsSource() || !filterSource)){
                        //Check if the source with this ID is already referenced:
                        SourceType source = document.getSource(
                                IDs.getSourceID(article.getArticleID().intValue()));
                        if (source == null){//If not, create and add it:
                                source = new Source(article);
                                document.addSource(source);
                        }
                        //Now, add source record to the list of source references
                        result.add(source);
                }
        }
        return result;
}
```

This list of the SourceType objects should be passed as the argument to the objects requiring the bibliographic references. For example, if a new DataType object is created, references may be attached to it in the following manner:

```
DataType quantity = new DataType(table.value, table.units);
quantity.addSources(Source.getSources(table.sourceRelation,request,true));
```

Here, “table” is an object of the database model, providing value and units fields plus the relation to the sources.

7.2 Attaching objects to the XSAMS Document tree

The interface **RequestInterface** provides the access to the XSAMS Document tree through the **XSAMSManager** interface. Node plugin may obtain the XSAMSManager by calling the **getXsamsManager()** method of the **RequestInterface**.

org.vamdc.xsams.XSAMSManager interface provides a handful of methods to add different branches to the XSAMS tree, getting them by known ID or iterating through all of them. For a full list of methods, consult the JavaDoc of the JAXB XSAMS library [XSAMSJavaDoc].

Most commonly used methods are:

- **String addSource(SourceType source);** returning the source identifier
- **String addElement(SpeciesInterface species);** returning the species identifier
- **int addStates(String speciesID,Collection<? extends StateInterface> states);** returning the number of added atomic or molecular states
- **boolean addProcess(Object process);** returning true if the process element was attached to the tree

for adding the sources, species, states and processes respectfully.

For each XSAMS block that has an identifier, a convenience method is implemented allowing to fetch the root element of the block by its string identifier. For example, for the sources block there exists a method **SourceType getSource(String sourceID)**.

A complete list of methods is available in the JavaDoc of the XSAMSManager interface [XSAMSJavaDoc].

7.3 Identifiers generation

Each major block of an XSAMS document has an unique identifier, an arbitrary alphanumeric string starting with a block-specific symbol.

To assure VAMDC-wide uniquiness of those identifiers, a node-specific prefix is inserted into every identifier string. For instance, that allows to merge the documents coming from the different databases.

In Java node software the identifiers are managed by a special class, **org.vamdc.xsams.IDs**. That class provides several static constants and methods:

- **String getID(char prefix, String suffix)** Most generic method, allowing to generate an arbitrary identifier. The allowed prefix values are enumerated as *public final static char* constants:
  - IDs.SOURCE
  - IDs.ENVIRONMENT
  - IDs.SPECIE
  - IDs.FUNCTION
  - IDs.METHOD
  - IDs.STATE
  - IDs.MODE
  - IDs.PROCESS
- **String getSourceID(int idSource)** ;

- **String getEnvID(int idEnv)** for the environment identifiers
- **String getFunctionID(int idFunction)** ;
- **String getMethodID(int idMethod)** ;
- **String getStateID(int EnergyTable, int Level)** ;
- **String getModeID(int molecule, int mode)** ;
- **String getSpecieID(int idSpecies)** ;
- **String getProcessID(char group, int idProcess)** ;

All those ID generation methods automatically add the configured node-specific ID prefix.

7.4 XSAMS JAXB convenience extensions

For convenience, all the XSAMS object classes were extended and grouped by the schema block into different packages :

- **org.vamdc.xsams.common** for elements used all around the schema
- **org.vamdc.xsams.environments** for elements from the Environments branch
- **org.vamdc.xsams.functions** for elements from the Functions branch
- **org.vamdc.xsams.methods** for elements from the Methods branch
- **org.vamdc.xsams.process** for elements from the Processes (collisions,transitions) branch
- **org.vamdc.xsams.sources** for elements from the Sources branch
- **org.vamdc.xsams.species** for elements from the Species (atoms, molecules, particles, solids) branch

Few value constructors were added:

- class **org.vamdc.xsams.species.molecules.ReferencedTextType**:

  ```
  public ReferencedTextType(String value);
  ```

  Creates a ReferencedTextType element with the defined value

- class **org.vamdc.xsams.sources.AuthorsType**:

  ```
  public AuthorsType(Collection<String> authors)
  public AuthorsType(String concatAuthors, String separator)
  ```

  First constructor creates Authors elemen with all authors from the passed collection, second one splits the first argument using the separator from the second one and puts the resulting strings into distinct Author records.

- class **org.vamdc.xsams.sources.AuthorType**:

  ```
  public AuthorType(String name)
  ```

  Creates a single Author element with the name from the argument.

- class **org.vamdc.xsams.common.TabulatedDataType**:

  ```
  public TabulatedDataType(String... CoordsUnits);
  public TabulatedDataType(Collection<String> columns);
  ```

  Constructors, defining multi-dimensional tables. Parameters passed define the units of axes, the last element of the collection or the last string define the units for Y (values). The *org.vamdc.xsams.common.TabulatedDataType* class contains a full set of methods for the XSAMS tables manipulation, so if you need to use them it is worth reading the XSAMS library JavaDoc [XSAMSJavaDoc]

- class **org.vamdc.xsams.common.DataType**:

```
public DataType(Double value,String units, AccuracyType accuracy, String comments);
public DataType(Double value,String units);
```

You will certainly use DataType objects, since almost any quantity in XSAMS is represented by them. Two constructors are provided, with parameter names speaking for themselves. Source references may be attached to created object later by calling the *addSource()* or *addSources()* methods.

- class **org.vamdc.xsams.common.ValueType**:

  ```
  public ValueType(Double value, String units);
  ```

  ValueType, used as often as the DataType, supports no source reference and is a simple extension of the Double type, providing the *units* attribute. Convenience constructor is also provided for it.

- class **org.vamdc.xsams.common.ChemicalElementType**:

  ```
  public ChemicalElementType(int charge, String symbol);
  ```

  Used in Atoms and Solids branches, ChemicalElementType has a convenience constructor consuming the atom nuclear charge and its chemical element symbol.

7.5 Case-By-Case generic builders

Molecular state quantum numbers in XSAMS are represented as additional XML sub-schemas, defining an element QNs with the ordered child quantum number elements. Each case has its own separate namespace, that means that Java JAXB mapping of each case would be in a separate package and the user would either require a generic builder using Java Reflection or have a builder for each case.

Since all cases are just combinations of roughly 30 quantum numbers, it was chosen to create an intermediate structure to contain them, together with the case identifier. The class name is **org.vamdc.xsams.util.StateCore**. It holds a collection of quantum numbers and other important state-related information.

Each quantum number is represented by the **org.vamdc.xsams.util.QuantumNumber** object. That object contains the value, optional label and mode index, plus the mandatory quantum number type.

Each case package is complemented with its own builder. The general case builder **org.vamdc.xsams.cases.CaseBuilder** accepts the **StateCore** object as a single parameter. Depending on the caseID parameter value, a specific case builder is called, returning the built tree. The identifier Case ID is the same as defined in the case-by-case documentation.

The following code illustrates the use of the **CaseBuilder**:

```
StateCore statedata = new BasecolStateCore(myetable, level);
MolecularStateType molecularState = new MolecularStateType();
// filling in other MolecularStateType fields is omitted
if (myrequest.checkBranch(Requestable.MoleculeQuantumNumbers))
        molecularState.getCases().add(CaseBuilder.buidCase(statedata));
```

Here, **BasecolStateCore** is a custom class that extends **StateCore**, providing a custom constructor to fill the fields from the Basecol Cayenne objects.

MolecularStateType is the autogenerated XSAMS JAXB mapping class that should be fed direcly to the XSAMS library by calling the:

```
RequestInterface.getXsamsroot().addState(speciesID, molecularState);
```

Please note that the element corresponding to the given speciesID should be attached to the XSAMS tree before attaching the state.

CHAPTER

EIGHT

VSS QUERY PARSING AND MAPPING

Vamdc nodes are queried using a common SQL-like keyword-based query language. A typical query looks like:

```
SELECT * WHERE (keyword1=value or keyword2=value2) and keyword3='value3'
```

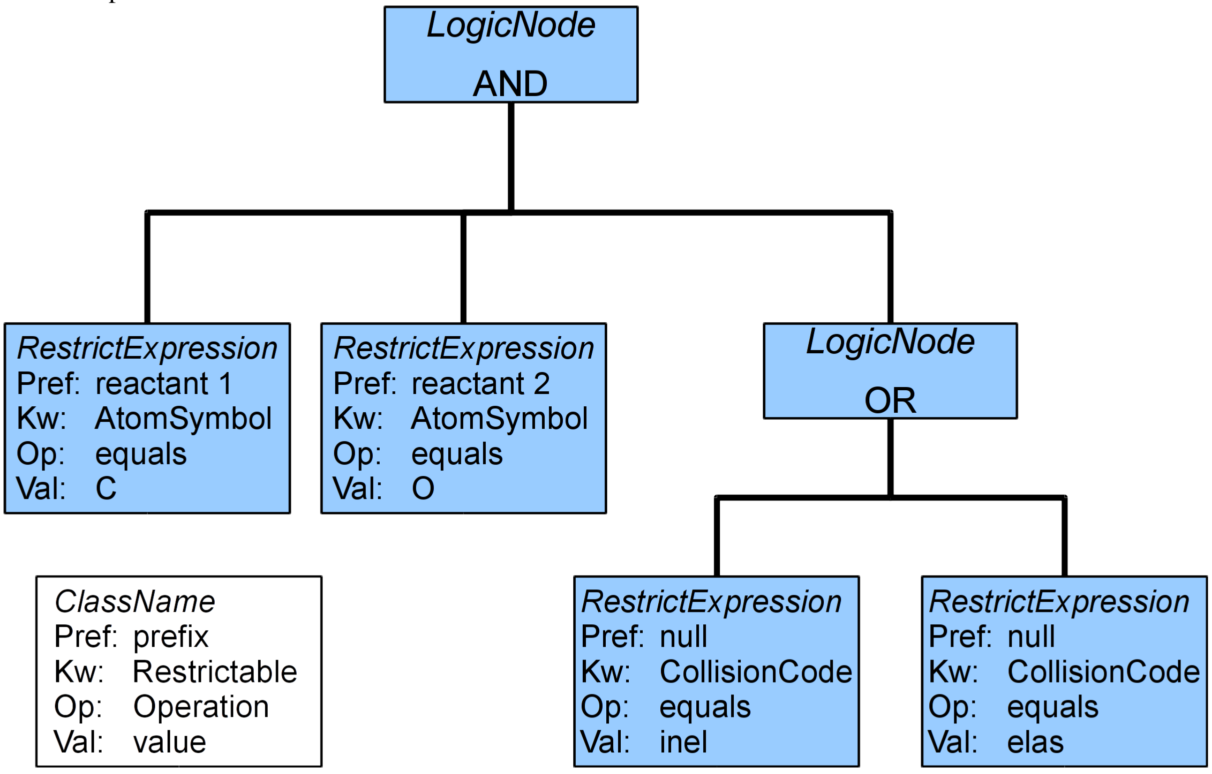
where the keywords correspond to the different parts of the XSAMS document and are defined in the VAMDC Dictionary [VAMDCDict] as Restrictable keywords. Since every VAMDC node has a specific database structure, the incoming query keywords need to be mapped to the database fields in order to fetch the data corresponding to the query. Java Node software tries to make the process of query mapping as simple and sophisticated as possible.

8.1 Query keywords tree

As a first step, on query reception the Java Node Software parses the query into a tree of objects using the **vamdctap-queryparser** library. Leaf nodes of that tree of objects represent the individual keyword expressions. The root node and the branches are reflecting the boolean relations between the leaves. For instance, a query:

```
SELECT * WHERE reactant1.AtomSymbol = 'C' AND reactant2.AtomSymbol = 'O'
AND (CollisionCode='inel' or CollisionCode='elas')
```

would map into the tree



8.2 QueryParser library interface

The QueryParser libary provides an interface *org.vamdc.tapservice.vss2*. **Query** providing several methods to access the incoming query elements.

8.2.1 Query

The methods to access the incoming query elements are:

- **public LogicNode getRestrictsTree()** is the main method, returning the root of the query tree.

  Accompanying are two methods, **getFilteredTree** and **getPrefixedTree**, returning the subsets.
- **public LogicNode getFilteredTree(Collection<Restrictable> allowedKeywords)** returns a subtree containing only the keywords present in the collection that is passed as a parameter.
- **public LogicNode getPrefixedTree(VSSPrefix prefix, int index)** returns a subtree containing only the keywords having the prefix and index that are passed to the method. If *null* is passed as a prefix, returned tree would only contain nodes that have a *null* prefix.
- **public Collection<Prefix> getPrefixes()** returns a collection of prefixes that are present in the query
- **public List<RestrictExpression> getRestrictsList()** returns a list of all the keywords that are present in the query. The logic of relations between the elements is lost.

8.2.2 LogicNode

The *LogicNode* interface represents a node of the query tree. **getOperator()** method provides access to the node operator (**OR**, **AND**, **NOT**), **getValues()** returns a collection of child nodes.

For the single-value operators like **NOT**, the **getValue()** method may be used to obtain the child element directly.

8.2.3 RestrictExpression

The leaf nodes of the logic tree are implementing the RestrictExpression interface, representing the query expressions.

The *RestrictExpression* interface is the extension of the *LogicNode* interface providing the **getOperator()**, **getValues()** and **getValue()** methods, as well as few additional methods:

- **public Prefix getPrefix()** a method returning the prefix used in the expression.
- **public Restrictable getColumn()** a method returning the Restrictable keyword used by the expression.

8.2.4 Prefix

Prefix is a simple class, keeping the **VSSPrefix** keyword of the dictionary, plus an integer index of the prefix.

- **int getIndex()** method provides access to the index, and
- **VSSPrefix getPrefix()** gives access to the prefix name.

8.3 Filtering logic

The algorithm implemented for the **getFilteredTree()** and **getPrefixedTree()** methods of the *Query* interface works the following way: It removes the irrelevant RestrictExpression objects from LogicNodes, than removes the Nodes of the tree that have no child expression elements.

For example, in the case of filtering by the prefix:

- Original query:

  ```
  select ALL where reactant1.AtomSymbol='C' and reactant1.AtomIonCharge=1
  and reactant2.AtomSymbol='H' and reactant2.AtomIonCharge=-1 and EnvironmentTemperature > 100
  ```

- Effective query for getPrefixedTree(VSSPrefix.REACTANT, 1):

  ```
  select ALL where reactant1.AtomSymbol='C' and reactant1.AtomIonCharge=1
  ```

- Effective query for getPrefixedTree(VSSPrefix.REACTANT, 2):

  ```
  select ALL where reactant2.AtomSymbol='H' and reactant2.AtomIonCharge=-1
  ```

- Effective query for getPrefixedTree(null, 0):

  ```
  select ALL where EnvironmentTemperature > 100
  ```

- Effective query for getFilteredTree(Collection<Restrictable>{AtomSymbol}) with a collection containing only the AtomSymbol element:

  ```
  select ALL where reactant1.AtomSymbol='C' and reactant2.AtomSymbol='H'
  ```

8.4 Query mapping scenarios

To perform queries on the actual database, the incoming VAMDC-TAP query needs to be adapted to the database structure. In the case of Apache Cayenne, *org.apache.cayenne.exp*.**Expression** object needs to be constructed, representing the query logic relative to the database primary table.

In this chapter the way to construct the query expressions from the incoming query is described.

8.4.1 Mapping of the LogicTree

Mapping of the LogicTree nodes is simple with one-to-one mapping of **AND**, **OR** and **NOT** operators to Cayenne Expression.andExp(), Expression.orExp(), Expression.notExp(), see the Cayenne Javadoc [CAYJAVADOC].

Usable example of such mapper is provided in *org.vamdc.tapservice.query.QueryMapper* class (vamdctap-querymapper library), that is bundled both with the TAPValidator and the node software.

8.4.2 Mapping of RestrictExpression elements

Mapping of the leaf nodes of the query tree, represented by the RestrictExpression elements, may be a bit more tricky. A lot of the information is contained in leaf nodes that should be mapped into the query logic:

- Keyword prefix
- Prefix index
- VAMDC dictionary Restrictable keyword
- comparison operator
- value or a set of values

VAMDC Restrictable keyword may correspond to one or several database fields. For example, let us have a database where all the species: particles, atoms and molecules are stored in a single table, where the inchikeys are defined for atoms and molecules, and there is a field indicating the species type. In this case the **MoleculeInchiKey** keyword in a query will map to two internal **Expression** constraints:

a constraint on the inchikey field of the table,

and a constraint indicating that the species is actually a molecule.

To correctly handle such a keyword we will need to join two Cayenne Expressions with the Expression.andExp operator, then add them to the mapped query tree.

Prefix and prefix index may also impose a check for a certain field, like if element is a reactant or product in a chemical reaction.

To handle the prefixes, it is possible to loop through the prefixes present in the query by using **Query.getPrefixes()** method. The second step would be to filter the incoming query tree by the prefix using the **Query.getPrefixedTree(...)** method, than map it to Cayenne Expressions, and finally join the obtained expressions with the Expression.andExp() method.

8.5 Query Mapping Library

As a part of the Java Node software, a Query Mapper library (**vamdctap-querymapper**) is provided. It is able to map the incoming query trees into cayenne Expression objects. Two interfaces and generic implementations within a package *org.vamdc.tapservice.querymapper* are provided:

- **KeywordMapper** defining an interface of a RestrictExpression mapper;
- **KeywordMapperImpl** a generic implementation, providing one-to-one mapping of Restrictable keywords to the database fields. No value transformation is performed. The node plugin may extend this class to implement the value translation, one-to-many fields mapping, or even the prefix-conditional mapping.
- **QueryMapper** defining the library main interface;
- **QueryMapperImpl** providing a generic implementation. That implementation keeps the references to all the defined **KeywordMapper** instances. It is capable of mapping the parsed query trees to Cayenne Expressions. Boolean logic of **LogicNode** tree is translated one-to-one by using the Apache Cayenne **Expression** *andExp()*, *orExp()* and *notExp()*. For leaf nodes the registered **KeywordMapper** instances are called to translate the **RestrictExpression** into the Cayenne Expression objects.

8.5.1 Using the querymapper library

From the plugin point of view the mapper library is used in the following way:

- A static instance of QueryMapper is initialized. For each supported Restrictable keyword a new mapper is added:

  ```
  public final static QueryMapper queryMapper= new QueryMapperImpl(){{
          this.addMapper(
                          new KeywordMapperImpl(Restrictable.IonCharge)
                          .addNewPath("symelementRel.elementRel.charge")
                          .addNewPath("partyRel.elementRel.charge")
                          );
  }};
  ```

  To define the database relations paths originating from different primary tables, subsequent calls to **addNewPath** method are used. Here for example the first path originates from the Species table, the second one originates from the Processes.

- If the advanced mapping is necessary, the class **KeywordMapperImpl** may be extended. Extension classes may add for example a possibility to map keywords to multiple fields, translate values from query units to database units.
- The **QueryMapper** implementation automatically handles a list of Restrictable keywords supported by the node. That list may be fetched by the **public Collection<Restrictable> getRestrictables()** method.
- The mapping of the incoming query trees or filtered subtrees is performed using the **QueryMapper** methods **mapAliasedTree(...)** or **mapTree(...)**. Cayenne **Expression** objects are produced as the output.

CHAPTER

NINE

QUERY METRICS SUPPORT

To give the estimation of the volume of data returned by the node for a query, the node software supports HEAD request queries. The parameter set of the HEAD request is the same as for the GET requests.

The VAMDC-specific HTTP headers that may be present in the response are the following:

- ***VAMDC-COUNT-SPECIES*** Total count of the atomic **Ion** and **Molecule** records with distinct SpecieID attribute.
- ***VAMDC-COUNT-ATOMS*** Count of the atomic **Ion** records with distinct SpecieID attribute.
- ***VAMDC-COUNT-MOLECULES*** Count of the **Molecule** records with distinct SpecieID attribute.
- ***VAMDC-COUNT-SOURCES*** Count of distinct **Source** records
- ***VAMDC-COUNT-STATES*** Count of distinct **State** records, both **AtomicState** and **MolecularState** combined
- ***VAMDC-COUNT-COLLISIONS*** Count of the **CollisionalTransition** elements of the **Processes** branch of XSAMS.
- ***VAMDC-COUNT-RADIATIVE*** Count of the **RadiativeTransition** elements of the **Processes** branch of XSAMS.
- ***VAMDC-COUNT-NONRADIATIVE*** Count of the **NonRadiativeTransition** elements of the **Processes** branch of XSAMS.
- ***Last-Modified*** **HTTP header can also be sent to client to indicate the time when the extracted** data was modified last time.

9.1 getMetrics(...) method

HTTP HEAD response may be produced without building the XSAMS document tree. For this purpose a dedicated plugin method is called by the node software for each incoming HEAD request.

:: public abstract Map<Dictionary.HeaderMetrics,Object> getMetrics(RequestInterface userRequest);

userRequest parameter has the same interface as the parameter of the plugin *buildXSAMS* method. Since the HEAD response will not transmit the XSAMS document body, there is no need to access the *XSAMSManager* object.

Typical logic of the method implementation would be the following:

- Translate the query using the same translation strategy as the builders use;
- Convert the query into the *SELECT Count(*) WHERE ...* using the *org.vamdc.tapservice.query.QueryUtil.countQuery(DataContext,SelectQuery)* static method;
- Add the obtained count() value along with the corresponding HTTP header to the map of result headers;

- If the obtained count() value is greater than zero, set the value of the *Last-Modified* header by using the **RequestInterface** *setLastModified(...)* method and *org.vamdc.tapservice.query.QueryUtil.lastTimestampQuery(...)* translator to obtain the value from the database last-modified date column.
- iterate over all primary tables if more than one primary table is used to query the database.

9.2 Sample implementation

Here follows the sample implementation from BASECOL database plugin

```
@Override
public Map<HeaderMetrics, Integer> getMetrics(RequestInterface request) {
        if (request.isValid() && checkRequest(request)){
                return Metrics.estimate(request);
        }
        return null;
}
```

and Metrics.estimate has the following implementation:

```
public static Map<HeaderMetrics, Object> estimate (RequestInterface request){
        Map<HeaderMetrics, Object> estimates = new HashMap<HeaderMetrics, Object>();

        //Estimate collisions
        Expression colExpression = CollisionalTransitionBuilder.getCayenneExpression(request);
        SelectQuery query=new SelectQuery(Collisions.class,colExpression);
        Long collisions = QueryUtil.countQuery((DataContext) request.getCayenneContext(), query);

        if (collisions>0){
                estimates.put(HeaderMetrics.VAMDC_COUNT_COLLISIONS, collisions.intValue());

                request.setLastModified(QueryUtil.lastTimestampQuery(
                                (DataContext) request.getCayenneContext(),
                                query,
                                "modificationDate"));
        }

        //Estimate species
        Expression spExpression = ElementBuilder.getExpression(request);
        SelectQuery spQuery=new SelectQuery(EnergyTables.class,spExpression);
        Long etables = QueryUtil.countQuery((DataContext) request.getCayenneContext(), spQuery);

        if (etables>0){
                estimates.put(HeaderMetrics.VAMDC_COUNT_SPECIES, etables.intValue());

                request.setLastModified(QueryUtil.lastTimestampQuery(
                                (DataContext) request.getCayenneContext(),
                                spQuery,
                                "modificationDate"));
        }

        return estimates;

}
```

Here, the getExpression(...) methods are the same translator methods as used in corresponding XSAMS builders.

CHAPTER

TEN

VAMDC-TAP NODE DEPLOYMENT

10.1 Install a Java application server

The Java implementation of the VAMDC-TAP node software is provided as a web application archive (.war) and is intended to be run under a Java application server like Apache Tomcat. For the server installation instructions refer to the server documentation.

10.2 Deploy the node software

Once the node plugin is tested with TAPValidator and working, a few steps are needed to install(deploy) a VAMDC node using the Java Node software.

1. Download the latest version of Java Node Software from the VAMDC site: http://www.vamdc.org/software/ What you need is a web application archive vamdctap-webservice-xxx.war
2. Deploy the downloaded .war file using your server default deploy method. (see the server documentation). The contents of the .war archive is unpacked to *webapps/vamdctap.../* by the server.
3. The Apache Cayenne configuration files need to be copied to WEB-INF/classes/ subdirectory of the unpacked web application archive. The cayenne project file needs to be renamed into **cayenne-project.xml** Database credentials can be changed in WEB-INF/classes/cayenne-project.xml or in dbcp.properties if you are using Apache DBCP for the database connection pooling.
4. Load the address *http://$BASEURL/config* to see the default configuration. To alter the options, a key-value pairs should be saved in a text file *WEB-INF/config/tapservice.conf*. For a full list of options and their desriptions please refer to the section *Node Configuration File*.
5. The node plugin and DAO jar files should be copied to *WEB-INF/lib/* directory of the deployed web application. **!WARNING!** Never try to copy those jars to the webserver or java system library paths. Such a configuration will never work, causing unexpected ClassCast exceptions.
6. The application or server should be reloaded to update the configuration and load the libraries.
7. Try to access the Capabilities and Availability endpoints of the service. They should be accessible through *http://$BASEURL/VOSI/capabilities* and *http://$BASEURL/VOSI/availability*. Availability status should be **Service is currently available: true**
8. **!WARNING!** Do a backup copy of all configuration files and .jar files that were put or adjusted in the deployed application folder, notably the node configuration files. All those files will be erased on every **vamdctap-webservice** war redeployment and should be recopied in place every time the Java Node Software web application is updated or relocated.
9. Once the deployment procedure is complete, the node operation should be tested using the TAPValidator application. In the TAPValidator configuration the network mode should be chosen and the capabilities endpoint address of the node should be indicated.

10.3 Node Configuration File

Java VAMDC-TAP node is configured through a single file, containing a set of key-value pairs.

The configuration may be altered by modifying the file *WEB-INF/config/tapservice.conf* in the web application root directory. Once the new parameters are set, the application should be reloaded to take the account of modifications.

The current node configuration may be retrieved by accessing the config endpoint: *http://host.name:8080/tapservice/config*. Here *host.name:8080/tapservice* is the url of the deployed web application.

10.3.1 Default configuration parameters

By default, the node parameters take the following values:

```
limits_enable=false
limit_states=-1
limit_processes=-1
selfcheck_interval=60
database_plug_class=org.vamdc.database.tap.OutputBuilder
dao_test_class=org.vamdc.database.dao.ClassName
xsams_id_prefix=DBNAME
baseurl=http://host.name:8080/tapservice#http://mirror.host/tapservice
xml_prettyprint=false
test_queries=select species where atomsymbol like ’%’;select * where inchikey=’UGFAIRIUMAVXCW-UHF
returnables=keyword1;keyword2;...
processors=ivo://vamdc/processor_1#ivo://vamdc/processor2
```

10.3.2 Detailed parameters description

- **limits_enable** = *(true|false)* enable output document element count limits
- **limit_states** = N - limit maximum output states count in document to N, “-1” disables the limit.
- **limit_processes** = N - limit maximum output processes count in document to N, “-1” disables the limit.
- **selfcheck_interval** = N interval in seconds between the node availability self checks. First check is initiated upon the request to /VOSI/availability endpoint. Background checks allow the accurate tracking of “upSince”, “backAt” and “downAt” time attributes.
- **database_plug_class** = *org.vamdc.database.tap.OutputBuilder* The name of the class implementing the *org.vamdc.tapservice.api.***DatabasePlugin** interface. An instance of that class is created on the web application startup. Methods of this class are invoked to construct a response for the incoming request.
- **dao_test_class** = *fully.qualified.apache.cayenne.dao.Object* The name of a Cayenne DAO class, used for the node availability checking. A table behind that class should have more than 10 records. This option may be omitted but in that case the availability endpoint will not work properly.
- **xsams_id_prefix** = *DBNAME* Prefix for XSAMS library id generator org.vamdc.xsams.util.IDs, used to produce all XML id/idRef references. Each node needs to have it’s own prefix to maintain globall uniquiness of identifiers in XSAMS documents.
- **baseurl** = *http://host.name:8080/tapservice* Base url used in VOSI/capabilities output, must contain globally accessible URL pointing to the VAMDC-TAP service web application root. Multiple addresses may be specified to indicate mirror nodes, separated by # symbol. The first address must point to the node itself.
- **xml_prettyprint** = *(true|false)* Produce pretty-printed XML documents or output everything in a single line of text with no linefeeds. Defaults to false, enabling it increases the size of output XML document by ~20%
- **test_queries** = *select species where atomsymbol like ‘%’;* semicolon-separated list of valid test queries for the node. It must contain only valid queries that demonstrate the full functionality of the node. On the other

hand such queries must produce compact documents, since those queries would be used for periodic node testing.

- **returnables** a semicolon-separated list of Returnable keywords that will be shown in the Capabilities endpoint output. May be left empty.
- **processors** a list of IVOA identifiers of the preferred XSAMS processors. This list is used by the vamdc portal to suggest the processors. Processor identifiers may be obtained from the VAMDC registry using the TAPValidator application (starting from version 12.07r2).

  To obtain the configuration parameter, open the TAPValidator, in the menu bar select Tools->Processors. A window will appear, containing the table of the registered processors. Select the lines while holding the ctrl key. Press the "Copy Selected" button. A text line containing the processors configuration option is copied to clipboard and may be pasted directly into the configuration file using your preferred text editor.

10.4 Cayenne configuration using DBCP

To avoid database connection time-out errors, Apache *commons-dbcp* library should be used in junction with Apache Cayenne. Configuration change for this case is simple and straight-forward. **vamdctap-webservice** application archive already comes with bundled *commons-dbcp* jar.

- in the file cayenne-project.xml the *factory* attribute of the **node** element should be changed to org.apache.cayenne.conf.DBCPDataSourceFactory.
- dbcp.properties configuration file should be put next to the cayenne-project.xml in the classes directory. the following parameters should be put into the file:

```
cayenne.dbcp.driverClassName=com.mysql.jdbc.Driver
cayenne.dbcp.url=jdbc:mysql://hostname:port/databasename
cayenne.dbcp.username=databaseUserName
cayenne.dbcp.password=databasePassword
```

Other DBCP parameters may be adjusted, please consult http://commons.apache.org/dbcp/configuration.html for more information.

10.5 Database updates and cache

Java node software maintains its own database cache. If database fields are updated, this cache needs to be purged. To force node to purge its caches, request to $BASEURL/clear_cache resource needs to be sent. The full URL will be http://host.name:8080/tapservice/clear_cache. Result document contains a single line of text, indicating the number of records that were contained in the cache.

This URL should be called every time the database contents is updated. It may be accessed either manually, included as an iframe in the node database administration interface, or accessed by a special script that tracks database modifications in some way.

10.6 Node mirroring

The best way to set up node mirrors is to configure database replication and deploy an instance of the node software on each mirror.

Deployment procedure of node software on master server and mirrors is the same. The only difference will be the order of the addresses in the **baseurl** configuration parameter on each of the mirrors.

10.6.1 Mysql master server configuration

On master server we need to enable binary logging in my.cnf:

```
[mysqld]:
server-id = 1
log-bin = /var/lib/mysql/mysql-bin
replicate-do-db = databasename
bind-address = 0.0.0.0
```

and add user with replication privileges in mysql console:

```
mysql@master> GRANT replication slave ON "databasename".* TO "replication"@"mirror.ip.or.hostname
        IDENTIFIED BY "password";
```

mysql service needs to be restarted after that.

After server restart we need to create a database dump:

> mysql@master> FLUSH TABLES WITH READ LOCK; mysql@master> SET GLOBAL read_only = ON; mysql@master> SHOW MASTER STATUSG
>
> #mysqldump -u root -p databasename | bzip2 -9 -c - > database_dump.sql.bz2
>
> mysql@master> SET GLOBAL read_only = OFF;

Here we need to note **File** and **Position** values from the mysql command *Show Master Status*.

10.6.2 Mysql slave configuration

On a slave (replica) server we need to set up the following things:

import mysql dump for database:

```
#bzip2 -d -c database_dump.sql.bz2 | mysql -u root -p databasename
```

In my.cnf:

```
[mysqld]:
server-id = 2
relay-log = /var/lib/mysql/mysql-relay-bin
relay-log-index = /var/lib/mysql/mysql-relay-bin.index
replicate-do-db = testdb
```

restart mysql service and start replication:

```
mysql@replica> CHANGE MASTER TO MASTER_HOST = "master.ip.or.host", MASTER_USER = "replication",
MASTER_PASSWORD = "password", MASTER_LOG_FILE = "mysql-bin.000003", MASTER_LOG_POS = 98;
mysql@replica> start slave;
```

where MASTER_LOG_FILE and MASTER_LOG_POS parameters we take from the *SHOW MASTER STATUS G* mysql command on master server.

Then we may see the slave server status by issuing mysql command:

```
mysql@replica> SHOW SLAVE STATUS\G
```

Following status parameters are important and indicated values show that replication is working properly:

- **Slave_IO_State**: Waiting for master to send event
- **Slave_IO_Running**: Yes
- **Slave_SQL_Running**: Yes
- **Seconds_Behind_Master**: 0

Changing **Read_Master_Log_Pos** parameter value may indicate that cache of node software on the mirror needs to be purged. A script can be set up to track this parameter, if no other mean of cache invalidation is used.

In detail mysql replication is described in the official manual: http://dev.mysql.com/doc/refman/5.5/en/replication.html

10.7 Node registration

To update the node registration to include the mirror nodes, two steps are needed:

- In the configuration of the main node and all mirrors the **baseurl** parameter should be set up to include the node and mirrors, separated with hash (#) symbol. On mirror nodes, the url of the mirror itself should be the first in that list. Java node web application should be reloaded to update the configuration.
- Registry record of the node should be updated with new Capabilities including new mirror.

In any case for the registry update please contact the VAMDC registry maintainer via support@vamdc.org.

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