



CLC **Server**

Administrator

USER MANUAL

Administrator Manual for
CLC Server 21.0.4
Windows, macOS and Linux

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This software is for research purposes only.

QIAGEN Aarhus
Silkeborgvej 2
Prismet
DK-8000 Aarhus C
Denmark



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Chapter 1

Introduction

Welcome to *CLC Server 21.0.4*, a central element of the CLC product line enterprise solutions.

The latest version of the user manual can also be found in pdf format at <https://digitalinsights.qiagen.com/technical-support/manuals/>.

You can get an overview of the server solution in figure 1.1. The software depicted here is for research purposes only.

Using a server means that data can be stored centrally and analyses run on a central machine rather than a personal computer. After logging into the CLC Server from a Workbench, data on the server will be listed in the Workbench navigation area and analyses can be started as usual. The key difference is that when you are logged into a CLC Server from a Workbench, you will be get the choice of where to run the analysis: on the Workbench or on the CLC Server.



Figure 1.1: An overview of the server solution. Note that not all features are included with all license models.

1.1 System requirements

The system requirements of *CLC Server* are:

Server system

- Windows 7, Windows 8, Windows 10, Windows Server 2012, Windows Server 2016 and Windows Server 2019
- Mac: OS X 10.10, 10.11 and macOS 10.12 through 11.2 The software is expected to run without problems on more recent macOS releases, but we do not guarantee this.
- Linux: RHEL 7 and later, SUSE Linux Enterprise Server 12 and later. The software is expected to run without problem on other recent Linux systems, but we do not guarantee this. To use BLAST related functionality, libnsl.so.1 is required.
- 64 bit
- For CLC Server setups that include job nodes and grid nodes, those nodes must run the same type of operating system as the master CLC Server.

- File system that supports file locking

Server hardware requirements

- Intel or AMD CPU required
- Computer power: 2 cores required. 8 cores recommended.
- Memory: CLC Genomics Server: 4 GB RAM required, 16 GB RAM recommended.
- Disk space: 500 GB required. More needed if large amounts of data are analyzed.

Special memory requirements for working with genomes

The numbers below give minimum and recommended amounts for systems running mapping and analysis tasks. The requirements suggested are based on the genome size.

- **E. coli K12 (4.6 megabases)**
 - Minimum: 2 GB RAM
 - Recommended: 4 GB RAM
- **C. elegans (100 megabases)** and **Arabidopsis thaliana (120 megabases)**
 - Minimum: 2 GB RAM
 - Recommended: 4 GB RAM
- **Zebrafish (1.5 gigabases)**
 - Minimum: 2 GB RAM
 - Recommended: 4 GB RAM
- **Human (3.2 gigabases)** and **Mouse (2.7 gigabases)**
 - Minimum: 6 GB RAM
 - Recommended: 8 GB RAM

Special requirements for de novo assembly

De novo assembly may need more memory than stated above - this depends both on the number of reads and the complexity and size of the genome. See http://resources.qiagenbioinformatics.com/white-papers/White_paper_on_de_novo_assembly_4.pdf for examples of the memory usage of various data sets.

Special requirement for the shared filesystem used by the job node setup or grid integration

The file locking mechanism is required to ensure that all nodes see the latest version of the data stored on the shared filesystem.

Special requirements for containerized external applications

Containerized external applications¹ are supported for Unix images run on Unix hosts only. Windows-based images and Windows hosts are not supported. Standard external applications are supported for any CLC Server setup.

¹Containerized external applications were introduced in CLC Server 21.0.

1.2 Licensing

Three kinds of license can be involved in running analyses on the *CLC Server*.

- **A license for the server software itself.** This is needed for running analyses via the server. The license will allow a certain number of open sessions. This refers to the number of active, individual log-ins from server clients such as Workbenches, the Command Line Tools, or the web interface to the server. The number of sessions is part of the agreement with QIAGEN when you purchase a license. Information about downloading and installing server licenses is provided in the Installation chapter, in section 2.6.
- **A license for the Workbench software.** CLC Workbenches are client software used to launch analyses on the server and to view the results. Find the user manuals and deployment manual for the Workbenches at <https://digitalinsights.qiagen.com/technical-support/manuals/>.
- **A network license if you will be submitting analyses to grid nodes.** This is explained in detail in section 6.3.5.

1.3 CLC Genomics Server

The *CLC Genomics Server* is shipped with the following tools and analyses that can all be started from *CLC Genomics Workbench* and *CLC Server Command Line Tools*:

- Import
- Export
- Search for Reads in SRA
- Download Genomes and References management
- Classical Sequence Analysis
 - Create Alignment
 - K-mer Based Tree Construction
 - Create Tree
 - Model Testing
 - Maximum Likelihood Phylogeny
 - Extract Annotations
 - Extract Sequences
 - Motif Search
 - Translate to Protein
 - Convert DNA to RNA
 - Convert RNA to DNA
 - Reverse Complement Sequence
 - Find Open Reading Frames

- Download Pfam Database
 - Pfam Domain Search
- Molecular Biology Tools
 - Assemble Sequences
 - Assemble Sequences to Reference
 - Secondary Peak Calling
 - Find Binding Sites and Create Fragments
 - Add attB Sites
 - Create Entry clone (BP)
 - Create Expression clone (LR)
- BLAST
 - BLAST
 - BLAST at NCBI
 - Download BLAST Databases
 - Create BLAST Database
- Track Tools
 - Merge Annotation Tracks
 - Convert to Tracks
 - Convert from Tracks
 - Remove Homozygous Reference Variants
 - Annotate with Overlap Information
 - Filter Annotations on Name
 - Filter Based on Overlap
 - Create GC Content Graph Tracks
 - Create Mapping Graph Tracks
 - Identify Graph Threshold Areas
- Prepare Sequencing Data
 - QC for Sequencing Reads
 - Trim Reads
 - Demultiplex Reads
- Resequencing Analysis
 - Map Reads to Reference
 - Local Realignment
 - Merge Read Mappings
 - Remove Duplicate Mapped Reads

- Extract Consensus Sequence
 - Identify Known Mutations from Sample Mappings
 - Basic Variant Detection (Variant Detectors)
 - Fixed Ploidy Variant Detection (Variant Detectors)
 - Low Frequency Variant Detection (Variant Detectors)
 - Copy Number Variant Detection (CNVs)
 - InDels and Structural Variants
 - QC for Targeted Sequencing
 - QC for Read Mapping
 - Whole Genome Coverage Analysis
 - Filter on Custom Criteria
 - Filter against Known Variants
 - Remove Marginal Variants
 - Remove Variants Present in Control Reads
 - Annotate from Known Variants
 - Remove Information from Variants
 - Annotate with Conservation Scores
 - Annotate with Exon Numbers
 - Annotate with Flanking Sequences
 - Identify Shared Variants
 - Identify Enriched Variants in Case vs Control Samples
 - Trio Analysis
 - Amino Acid Changes
 - Predict Splice Site Effect
 - GO Enrichment Analysis
 - Download 3D Protein Structure Database
 - Link Variants to 3D Protein Structure
- RNA-Seq Analysis
 - RNA-Seq Analysis and Small RNA Analysis
 - PCA for RNA-Seq
 - Differential Expression in Two Groups
 - Differential Expression for RNA-Seq
 - Create Heat Map for RNA-Seq
 - Create Expression Browser
 - Create Venn Diagram for RNA-Seq
 - Gene Set Test
 - Microarray Analysis

- Create Box Plot
- Hierarchical Clustering of Samples
- Principal Component Analysis
- Empirical Analysis of DGE
- Proportion-based Statistical Analysis
- Gaussian Statistical Analysis
- Create MA Plot
- Create Scatter Plot
- Create Histogram
- Epigenomics Analysis
 - Transcription Factor ChIP-Seq
 - Annotate with Nearby Gene Information
 - Map Bisulfite Reads to Reference
 - Call Methylation Level
 - Create RRBS-fragment Track
- De Novo Sequencing
 - De Novo Assembly
 - Map Reads to Contigs
- Utility Tools
 - Extract Annotations
 - Sample Reads
 - Extract Reads
 - Merge Overlapping Pairs
- Legacy Tools
 - Compare Sample Variant Tracks
 - Remove Reference Variants
 - Roche 454
 - Create Combined RNA-Seq Report
 - Create Track from Experiment
 - Extract and Count
 - Annotate and Merge Counts

The functionality of the *CLC Genomics Server* can be extended by installation of Server plugins. The available plugins can be found at <https://digitalinsights.qiagen.com/products-overview/plugins/>.

Latest improvements

CLC Genomics Server is under constant development and improvement. A detailed list that includes a description of new features, improvements, bugfixes, and changes for the current version of *CLC Genomics Server* can be found at:

<https://digitalinsights.qiagen.com/products/qiagen-clc-genomics-server/latest-improvements/current-line/>.

Chapter 2

Installation

2.1 Quick installation guide

The following describes briefly the steps needed to set up *CLC Genomics Server* with links out to more detailed explanations for each step.

If you are looking for how to set up a *CLC Network License Manager*, instructions can be found in the *CLC Network License Manager* manual.

If you are going to set up execution nodes as well, please read section 6 first.

1. Download and run the server software installer file. When prompted during the installation process, choose to start the server (section 2.2).
2. Install a license for the software. (section 2.6).
3. Restart the server (section 2.7).
4. Ensure the necessary port is open for access by client software for the server. The default port is 7777 .
5. Log into the server web administrative interface using a web browser using the username **root** and password **default** (section 3).
6. Change the root password (section 4.1).
7. Configure the authentication mechanism and optionally set up users and groups (section 4.2).
8. Add data locations (section 3.2).
9. Check your server setup using the **Check set-up** link in the upper right corner as described in section 15.1.
10. Your server should now be ready for client software to connect to and use.

2.2 Installing and running the Server

Getting the *CLC Server* software installed and running involves, at minimum, these steps:

1. Install the software.
2. Ensure the necessary port in the firewall is open.
3. Install a license.
4. Start the Server and/or configure it as a service.

All these steps are covered in this section of the manual.

Further configuration information, including for job nodes, grid nodes, and External Applications, are provided in later chapters.

Installing and running the *CLC Server* is straightforward. However, if you do run into problems, please refer to the troubleshooting chapter [15](#).

2.2.1 Installing the Server software

The installation can only be performed by a user with administrative privileges. On some operating systems, you can double click on the installer file icon to begin installation. Depending on your operating system you may be prompted for your password (as shown in figure [2.1](#)) or asked to allow the installation to be performed.

- On Windows 8 and Windows 7, you will need to right click on the installer file icon, and choose to **Run as administrator**.
- For the Linux-based installation script, you would normally wish to install to a central location, which will involve running the installation script as an administrative user - either by logging in as one, or by prefacing the command with `sudo`. Please check that the installation script has executable permissions before trying to execute it.



Figure 2.1: Enter your password.

Next, you will be asked where to install the server (figure [2.2](#)). If you do not have a particular reason to change this, simply leave it at the default setting. The chosen directory will be referred to as the *server installation directory* throughout the rest of this manual.

The installer allows you to specify the maximum amount of memory the *CLC Server* will be able to utilize (figure [2.3](#)). The range of choice depends on the amount of memory installed on your system and on the type of machine used. If you do not have a reason to change this value you should simply leave it at the default setting.

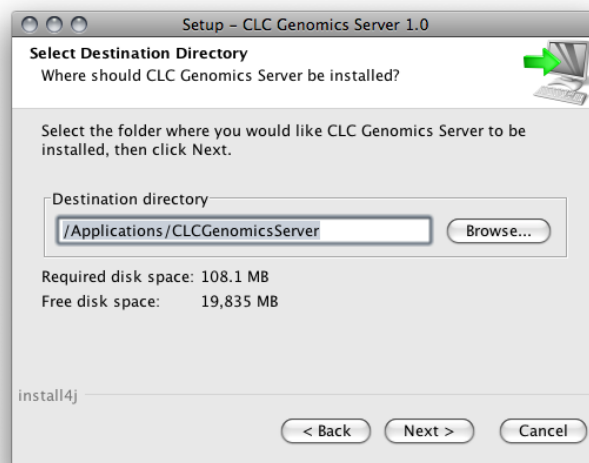


Figure 2.2: Choose where to install the server. Exemplified here with **CLC Genomics Server**

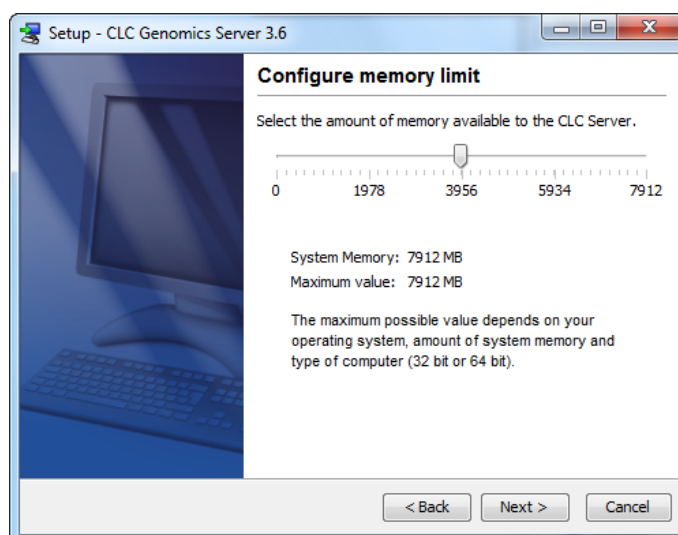


Figure 2.3: Choose the maximum amount of memory used by the server.

If you are installing the Server on a Linux system, you are offered the option to specify a user account that will be used to run the *CLC Server* process. Having a specific, non-root user for this purpose is generally recommended. On a standard setup, this would have the effect of adding this username to the service scripts, which can then be used for starting up and shutting down the *CLC Server* service and setting the ownership of the files in the installation area. Downstream, the user running the *CLC Server* process will own files created in File Locations, for example, after data import or data analyses.

If you are installing the server on a Windows system you will be able to choose if the service is started manually or automatically by the system.

The installer will now extract the necessary files.

On a Windows system, if you have chosen that the service should be started automatically, the service should also start running at this point. On Linux or Mac, if you have chosen the option to start the system at the end of installation, the service should also have started running. Please

note that if you do not already have a license file installed, then the *CLC Server* process will be running in a limited capacity at this point. Downloading a license is described in section 2.6.

Information on stopping and starting the *CLC Server* service is provided in section 2.7.

2.3 Installation modes - console and silent

Two installation modes are available to support efficient installation of the Workbench software.

- **Console mode** This mode is particularly useful when installing Workbenches onto remote systems. On Linux, this mode is enabled by using the option `-c` when launching the installer from the command line. On Windows the option is `-console`.
- **Silent mode** This mode supports hands-off installation. Default answers to all prompts are used, although a non-default installation directory can be specified if desired (see below). Silent mode is activated using the `-q` parameter when launching the installer from the command line. On Windows, the `-console` option can be appended after `-q`, that is, as the second parameter, to ensure output to the console.

If desired, you can **specify the directory to install the software to** when running the installer in silent mode. Do this adding the `-dir` option to the command line.

On Windows, the `-console` and the `-dir` options only work when the installer is run in silent mode.

The following is an example of a command that would install a Workbench into the directory "c:\bioinformatics\clc" on a Windows system using silent mode with console output :

```
CLCMainWorkbench_8_0.exe -q -console -dir "c:\bioinformatics\clc"
```

On a Linux system, a similar command to install into the directory "/opt/clcgenomicsworkbench11" could look like:

```
./CLCGenomicsWorkbench_11_0_1_64.sh -c -q -dir /opt/clcgenomicsworkbench11
```

The `-q` and the `-console` options work for the uninstall program as well.

2.4 Upgrading an existing installation

For a single *CLC Server*, the steps we recommend when upgrading to a new version are:

- Stop the *CLC Server* service after making sure that nobody is using the server. Mechanisms to help with this, including sending a message to users logged into the *CLC Server*, can be found in section 7.3. Getting information about who is logged in is described in section 7.1.
- Install the *CLC Server* software in the same directory the existing version was installed in. All settings will be maintained, for example, the locations data are stored, Import/Export directories, BLAST database locations, Users and Groups, and External Application settings.

If you have a CLC Job Node setup, you will also need to upgrade the *CLC Server* software on each job node. Upgrading the software itself on each node is all you need to do. Configurations for job nodes, as well as new or updated plugins, are pushed to them by the master node.

When upgrading between major versions, there are extra steps to be taken. These are described in section [2.4.1](#)). Major version lines are denoted by the first number in the version. For example, upgrading from software with version 10.0 to version 11.0 involves an upgrade to a new major version line.

2.4.1 Upgrading between major versions

There are a few extra steps to take beyond those outlined in section [2.4](#) when upgrading to a new major version line.

- An updated license file needs to be downloaded (see section [2.6](#)) and installed.
- Old license files should be deleted. License files can be found in a folder called "licenses" under the installation area of the *CLC Server*.
- The *CLC Server* service needs to be restarted.
- All users of client software (CLC Workbenches and the CLC Server Command Line Tools) must upgrade their software. Corresponding and compatible software versions are listed at the bottom of the Latest Improvement listings for a given server version. e.g. for the latest release, this can be found at: <https://digitalinsights.qiagen.com/products/qiagen-clc-genomics-server/latest-improvements/current-line/>.
- All plugins installed on the *CLC Server* need to be updated. See section [10](#).
- **On job nodes**, any new tools included in the server upgrade will need to be enabled for the nodes you wish them to be run on. New tools are initially disabled on all job nodes to avoid interfering with a setup where certain nodes are dedicated to running specific types of jobs. Read more about enabling tools on job nodes in section [6.2.2](#).

Important note when upgrading on macOS to CLC Genomics Server 11.0 or higher from earlier major release lines A flag in the `CLCGenomicsServer.vmoptions` file must be removed when upgrading in place from CLC Genomics Server 10.x or earlier to CLC Genomics Server 11.x or later on macOS. Please delete "-d64" from the `CLCGenomicsServer.vmoptions` file, which can be found in the CLC Genomics Server installation area and then restart the CLC Genomics Server service. The -d64 option is not supported by recent versions of java. Its inclusion in the `vmoptions` file on macOS systems will stop the CLC Genomics Server 11.0, and any later versions, from starting up.

2.5 Allowing access through your firewall

By default, the server listens for TCP-connections on port 7777 (see section [3.5](#) for info about changing this).

If you are running a firewall on your server system you will have to allow incoming TCP-connections on this port before your clients can contact the server from a Workbench or web browser. Consult the documentation of your firewall for information on how to do this.

Besides the public port described above the server also uses an internal port on 7776. There is no need to allow incoming connections from client machines to this port.

2.6 Downloading a license

Licenses can be downloaded and installed by going to the **Extensions** (🔧) tab in the web administrative interface of the single server or master node, and opening the **Download License** tab.

To download and install a license, enter the Order ID supplied by QIAGEN into the Order ID field and click on the "Download and Install License..." button (figure 2.4). Please contact ts-bioinformatics@qiagen.com if you have not received an Order ID.

The *CLC Server* must be restarted for the new license to take effect. Details about restarting can be found in section 2.7.1.

Each time you download a license file, a new file is created in the `licenses` folder under the *CLC Server* installation area. *If you are upgrading* an existing license file, *delete the old file* from this area before restarting..

If you are working on a system that does not have access to the external network, then please refer to section 2.6.1.

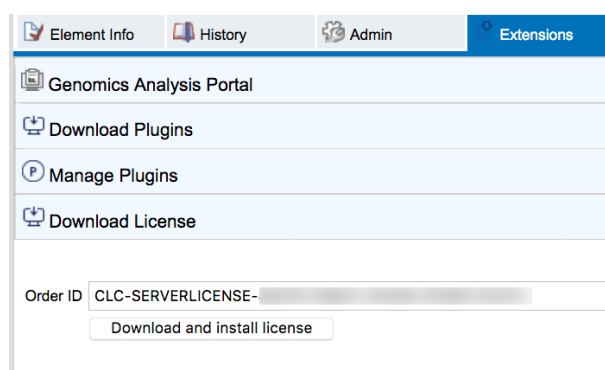


Figure 2.4: License management is done under the Extensions tab.

2.6.1 Download a static license on a non-networked machine

Follow the steps below to download a static license for a server machine that does not have direct access to the external network.

- Determine the host ID of the machine the server software will be running on. This can be done by running the back-end license download tool, which prints the host ID of the system to the terminal. The download tool is located in the installation folder of the *CLC Server*. The tool name depends on the system you are working on:
 - Linux: `downloadlicense`

- Mac: `downloadlicense.command`
- Windows: `licensedownload.bat`

In the case of a job or grid node setup, the host ID should be for the machine that will act as the *CLC Server* master node.

- Make a copy of this host ID such that you can use it on a machine that has internet access.
- Go to a computer with internet access, open a browser window and go to the server license download web page:

<https://secure.clcbio.com/LmxWSv3/GetServerLicenseFile>

For licenses for server extensions, the license download page is:

<https://secure.clcbio.com/LmxWSv3/GetLicenseFile>

- Paste in your license order ID and the host ID that you noted down earlier into the relevant boxes on the webpage.
- Click on 'download license' and save the resulting `.lic` file.
- On the machine with the host ID you specified when downloading the license file, place the license file in the folder called 'licenses' in the *CLC Server* installation directory.
- Restart the *CLC* software.

2.7 Starting and stopping the server

2.7.1 Microsoft Windows

On Windows based systems the *CLC Server* can be controlled through the *Services* control panel.

The service is named *CLC Genomics Server: CLCGenomicsServer*

Choose the service and click the start, stop or restart link as shown in figure 2.5.

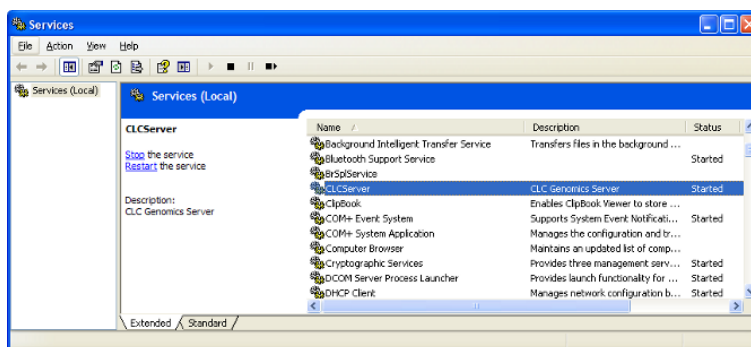


Figure 2.5: Stopping and restarting the server on Windows by clicking the blue links.

Once your server is started, you can use the Admin tab on the server web interface to manage your server operation (see section 7).

2.7.2 macOS

On macOS the server can be started and stopped from the command line.

Open a terminal and navigate to the *CLC Server* installation directory. Once there, the server can be controlled with the following commands.

Remember to replace *CLCServer*, in the commands listed below, with the name from the *CLC Genomics Server*: `CLCGenomicsServer`

To start the server run the command:

```
sudo ./CLCServer start
```

To stop the server run the command:

```
sudo ./CLCServer stop
```

To view the current status of the server run the command:

```
sudo ./CLCServer status
```

You will need to set this up as a service if you wish it to be run that way. Please refer to your operating system documentation if you are not sure how to do this.

Once your server is started, you can use the Admin tab on the server web interface to manage your server operation (see section 7).

2.7.3 Linux

You can start and stop the *CLC Server* service from the command line. You can also configure the service to start up automatically after the server machine is rebooted.

During installation of the *CLC Server* a service script is placed in `/etc/init.d/`.

This script will have a name reflecting the server solution, and it includes the name of the custom user account specified during installation for running the *CLC Server* process.

Starting and stopping the service using the command line:

To start the *CLC Server*:

```
sudo service CLCGenomicsServer start
```

To stop the *CLC Server*:

```
sudo service CLCGenomicsServer stop
```

To restart the *CLC Server*:

```
sudo service CLCGenomicsServer restart
```

To view the status of the *CLC Server*:

```
sudo service CLCGenomicsServer status
```

Start service on boot up:

On Red Hat Enterprise Linux and SuSE this can be done using the command:

```
sudo chkconfig CLCGenomicsServer on
```

How to configure a service to automatically start on reboot depends on the specific Linux distribution. Please refer to your system documentation for further details.

Troubleshooting

If the *CLC Server* is run as a service as suggested above, then the files in the installation area of the software and the data files created after installation in *CLC Server File Locations* will be owned by the user specified to run the *CLC Server* process. If someone starts up the *CLC Server* process as root (i.e. an account with super-user privileges) then the following steps are recommended to rectify the situation:

1. Stop the *CLC Server* process using the script located within the installation area of the *CLC Server* software. You can do that using the full path to this script, or by navigating to the installation area and running:

```
sudo ./CLCGenomicsServer stop
```

2. Change ownership recursively on all files in the installation area of the software and on all areas specified as *Server File Locations*.
3. Start the *CLC Server* service as the specified user by using the service script:

```
sudo service CLCGenomicsServer start
```

4. In case the server still fails to start correctly it can be started in the foreground with output being written to the console to help identify the problem. It is done by running:

```
sudo ./CLCGenomicsServer start-launched
```

Once your server is started, you can use the Admin tab of the web administrative interface to manage your server operation (see section 7).

2.8 Installing the database

This section pertains to the installation and configuration of an SQL database to store data imported into the *CLC Server*. This is relevant only if the database add-on has been purchased.

2.8.1 Download and install a Database Management System

If you do not have access to an existing installation of a Database Management System (*DBMS*) you will have to download and install one. *CLC Bioinformatics Database* can be used with a number of different *DMBS* implementations. Choosing the right one for you and your organization depends on many factors such as price, performance, scalability, security, platform-support, etc.

Information about the supported solutions are available via the links below.

- MySQL: <http://dev.mysql.com/downloads/>
- PostgreSQL: <http://www.postgresql.org/>

- Microsoft SQL Server: <http://www.microsoft.com/SQL/>
- Oracle: <http://www.oracle.com/>

You will need to make the appropriate JDBC driver available to the CLC Server. See section 17.2 for details and for additional configuration information for certain DBMSs.

2.8.2 Create a new database and user/role

Once your DBMS is installed and running you will need to create a database for containing your CLC data. We also recommend that you create a special database-user (sometimes called a database-role) for accessing this database.

Consult the documentation of your DBMS for information about creating databases and managing users/roles.

2.8.3 Initialize the database

Before you can connect to your database from a CLC Workbench or Server it must be initialized. The initialization creates the required tables for holding objects, and prepares an index used for searching. Initialization is performed with the CLC Bioinformatics Database Tool (see figure 2.6).

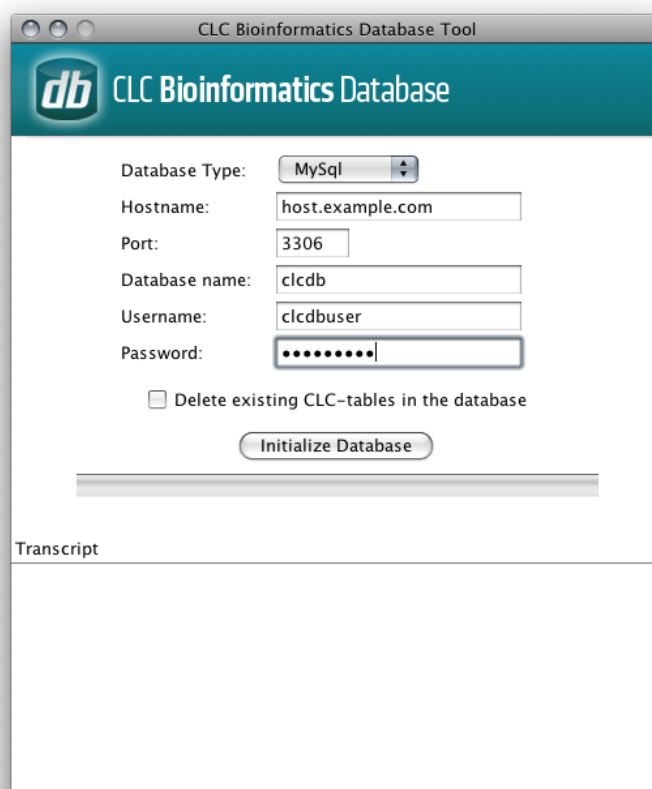


Figure 2.6: The CLC Bioinformatics Database tool

- Download the CLC Bioinformatics Database Tool from <https://digitalinsights.qiagen.com/products/clc-bioinformatics-database-tool-direct-download/>
- Install the CLC Bioinformatics Database Tool on a client machine, and start the program.
- Fill in the fields with the required information.
 - Hostname: The fully-qualified hostname of the server running the database.
NOTE: The same hostname must be used every time you connect to the database
 - Port: The TCP/IP listening port on the database server
 - Database name: The name of the database you created in the previous section
 - Username: the name of the user/role you created in the previous section
 - Password: the password for the user/role.
- To re-initializing an existing CLC database you must check the "Delete Existing..." checkbox.
NOTE: ANY DATA ALREADY STORED IN THE CLC DATABASE WILL BE DELETED.
- Click the Initialize Database button to start the process.

While the program is working the progress-bar will show the status and the transcript will show a log of actions, events and problems. If anything goes wrong, please consult the transcript for more information. If you need assistance, please contact ts-bioinformatics@qiagen.com, and include the contents of transcript.

If the initialization is successful, the status bar will display this message: *Database successfully initialized*. You can now close the CLC Bioinformatics Database Tool.

Chapter 3

Basic configuration

3.1 Logging into the administrative interface

The administrative interface for a running *CLC Server* is accessed via a web browser. Most configuration occurs via this interface. Simply type the host name of the server machine you have installed the *CLC Server* software on, followed by the port it is listening on. Unless you change it, the port number is 7777. An example would be

```
http://clccomputer:7777/ or http://localhost:7777/
```

The default administrative user credentials are:

- **User name:** root
- **Password:** default

Use these details the first time you log in. We recommend that you change this password.

Details of how to change the administrative user password is covered in section [4.1](#).

3.2 Adding locations for saving data

Before using the server for analysis, the areas for storing data imported into or created by the software need to be specified.

On most server setups, this involves configuring a file system location, as described in section [3.2.1](#).

For *CLC Server* setups with a license that supports the add-on *CLC Bioinformatics Database*, database locations can also be added, as described in section [3.2.4](#).

3.2.1 File system locations

Data storage configuration is done via the administrative web interface. When logged in as a user with administrative privileges, navigate to the *Admin* tab, click on the *Main configuration* tab, and then click on the **File system locations** heading to expand that section. See figure [3.1](#).

The options available when configuring a file system location are described below. After making any changes, click on the **Save Configuration** button at the bottom of this area. Any file system locations that have been added should then appear in the list at the left hand side of the web client.

Add a new file system location Click on the Add New File Location button and then specify the path to the folder where data imported into or created by the *CLC Server* will be stored. The path provided should point to an *existing* folder on the server machine that the user running the server process has read and write access to.

If a file system location with the name *CLC_References* is configured, users logged into a *CLC Server* from a *CLC Genomics Workbench* will be able to download data directly to this server area using the Workbench's Reference Data Manager tool. Special conditions apply to this file system location. These are outlined in section 3.2.2.

Enable or disable access for all users The checkbox to the left of each file system location is used to control whether or not it should be available to users. Access is enabled by default. For example, in a *CLC Workbench* connected to the *CLC Server*, each enabled location is visible in the **Navigation Area**. Unchecking this box and saving the configuration makes the location unavailable for use. Disabled locations are not be visible in a *CLC Workbench Navigation Area*.

Remove a file system location Clicking on the **Remove Location** button beside a particular file system location removes it from the *CLC Server*. The underlying folder and its contents are **not** deleted. To re-enable access via the *CLC Server*, simply configure the same folder as a file system location again.

Rebuild the index The *CLC Server* maintains an index of all the elements in a data location. This is used when searching for data. There is no need to re-index when adding a new area as a file system location. Rebuilding the index is described in more detail in section 3.2.5.

Enable permissions Permissions can be configured for all file system locations, except if they are named *CLC_References*. Changes to permissions settings first take effect after the server is restarted.

Group-based permissions After selecting this option, group-level read and write permissions can be configured for the file system location using a *CLC Workbench* client, as described in section 5.1. Until such access is granted, the file system location and its contents are available only to admin users.

User homes The file system location will be used for user home folders. These are top-level folders with names matching users' usernames. A user is granted write access only to the folder with a name matching their username. Admin users continue to have access to all folders.

- **Auto-create user homes** When selected, a user folder is created automatically by the *CLC Server* when a user first logs in. To create folders only for specific users, deselect this option and use the `mkdir` command of the *CLC Server Command Line Tools*, specifying the file system location as the target and providing a user's username as the name of the folder to create.
- **Allow global read access to user homes** When selected, all users are granted read access to all user home folders on this file system location. When not selected, users only have access to their own user home area.

The screenshot shows the 'Main configuration' window. Under the 'File system locations' section, there are three entries for file system locations:

- Location 1:** Path: . Permissions enabled: . Buttons: Remove Location, Rebuild Index.
- Location 2:** Path: . Permissions enabled: . Buttons: Remove Location, Rebuild Index.
 - Permissions configuration:
 - Group-based permissions:
 - User homes:
 - Auto-create user homes:
 - Allow global read access to user homes:
- Location 3:** Path: . Permissions enabled: . Buttons: Remove Location, Rebuild Index.
 - Permissions configuration:
 - Group-based permissions:
 - User homes:
 - Auto-create user homes:
 - Allow global read access to user homes:

Below the file system locations is the 'Data compression' section with a checkbox checked: 'Save CLC data elements in a compressed format. See the [manual](#) for more information.'

At the bottom, there are links for 'Import/export directories', 'Automatic recycle bin cleanup', 'Direct data transfer from client systems', and 'HTTP settings', followed by a 'Save Configuration' button.

Figure 3.1: File system location settings. The checkmark to the left of a configured location indicates it is available for use by those logged into the server. Permissions are not enabled by default. Internal data compression, which applies to all configured file system locations, is enabled by default.

When enabling the "User homes" option, please note that:

- Data elements stored directly under the file system location will be readable, but not writable, by all users. While it should only be possible for admin users to place data in this area, if the file system location was in use before the **User homes** option was selected, then existing data stored at the top level will be accessible to all users.
- Any folder at the top level of a CLC Server file system location with a name matching a user's username will be treated as a user home area, with read and write access granted to that user on that folder and its contents.

3.2.2 Reference data management

Using the Reference Data Manager of the CLC Genomics Workbench, data can be downloaded directly to a CLC Genomics Server file system location called *CLC_References*.

To enable this, a folder named *CLC_References* must be available on a file system the *CLC Server* has access to and which the user running the *CLC Server* process has read and write access to. That folder must then be configured as a file system location, as described in section 3.2.1.

Special conditions exist for a *CLC_References* file system location:

- All users logged into the CLC Genomics Server can see and use all data stored in *CLC_References*.
- All users logged into the CLC Genomics Server from a CLC Genomics Workbench can download data to this area using the Workbench Reference Data Manager.
- Only administrative users can delete data in this area using the CLC Genomics Workbench Reference Data Manager.
- No user, including admin users, can delete data stored in this area via the Navigation Area of the CLC Genomics Workbench.
- Data in this area can be deleted via the Element Info tab of the CLC Genomics Server web administrative interface.
- Custom permissions cannot be set on a *CLC_References* file system location. The checkbox enabling permissions should not be selected. If it is, only administrative users will be able to read or write to this area using the CLC Genomics Workbench Reference Data Manager.

Further information about the Reference Data Manager, including how to select to download to a server file location, can be found in the CLC Genomics Workbench manual: http://resources.qiagenbioinformatics.com/manuals/clcgenomicsworkbench/current/index.php?manual=References_management.html.

Important points about CLC Server file system locations

- Folders added as file system locations should be **dedicated for use** by the *CLC Server* and should be directly accessed only by the *CLC Server*.
- The underlying file system must support file locking.
- All the data written to file system locations by the *CLC Server* will be in *clc* format and will be owned by the user that runs the *CLC Server* process.
- Files should **not** be moved manually into folders designated as CLC Server file system locations, or their subfolders, for example using standard operating system's command tools, drag and drop, and so on.
- Areas designated as file system locations should **not** overlap. That is, if a folder has been designated as a file system location, it should not be a subfolder of another area also designated as a file system location, or vice versa. Overlapping file system locations lead to problems with data indexing, which in turn leads to problems finding the stored data. Further information about indexing can be found in section 3.2.5.

File locations for job node set-ups

When you have a job node set-up, all the job node computers need to have access to the same data location folder. This is because the job nodes will write files directly to the folder rather than passing through the master node (which would be a bottleneck for big jobs). Furthermore, the user running the server must be the same for all the job nodes and it needs to act as the same user when accessing the folder no matter whether it is a job node or a master node.

The data location should be added **after** the job nodes have been configured and attached to the master node. In this way, all the job nodes will inherit the configurations made on the master node.

One relatively common problem faced in this regard is *root squashing* which often needs to be disabled, because it prevents the servers from writing and accessing the files as the same user - read more about this at http://nfs.sourceforge.net/#faq_b11.

You can read more about job node setups in section 6.

3.2.3 Enabling and disabling internal compression of CLC data

CLC data stored using internal compression takes less space. An option is provided under the **Data compression** heading to turn off internal data compression. See figure 3.1. Enabling data compression may impose a performance penalty depending on the characteristics of the hardware used. This penalty is typically small, and we generally recommend that this option remains enabled.

This setting applies to all configured file system locations. Any change will apply to data imported into or created after the change is made. Existing data is not affected.

Internal data compression and data compatibility Internal compression was introduced with the CLC Genomics Server 11.0 and corresponding client software, the CLC Genomics Workbench 12.0 and CLC Main Workbench 8.1. Data imported into or created by these systems and newer versions are compressed by default. However, software older than this, including retired products, cannot read the compressed data format.

Data created using older versions of CLC software will not be stored in compressed format.

To facilitate sharing particular datasets with people using older versions of the software, an option is available when exporting the data to CLC or zip format to export without this compression.

3.2.4 Database locations

Adding an SQL database location for use by the *CLC Server* is possible after the relevant add-on has been purchased and a license supporting it has been installed.

Before adding a database location, you need to set up the database itself. This is described in section 2.8.

To set up a database location on the CLC Server,

- Open a web browser and navigate to the web administrative interface.
- Go to the *Admin* tab and open the *Main configuration* section.

- Under the **Database locations** heading, click the **Add New Database Location** button. This pops a window like that shown in figure 3.2.
- To configure the database location, enter the host and port information and select the database type. The *Database type* drop down list contains the types for which drivers are available. A connection string is generated from this. A custom connection string can be entered instead. Add the user name and password information for the user role on your Database Management System (DBMS), see section 2.8.

Figure 3.2: Adding a new database location. Here, two drivers are available to the CLC Server, a MySQL driver and an Oracle driver.

If an Oracle database driver is available to the CLC Server, two items will be presented in the Database type drop down list, as shown in figure 3.2. The one shown as "Oracle" is the traditional one, which uses the SID style (e.g. `jdbc:oracle:thin:@[HOST][:PORT]:SID`). The other, "Oracle Service", uses the thin-style service name (e.g. `jdbc:oracle:thin:@//[HOST][:PORT]/SERVICE`).

- Click the *Save Configuration* button to save the configuration.

The newly added database location should now appear in the **Navigation Area** in the left hand side of the window.

3.2.5 Rebuilding the index

The server maintains an index of all the elements in the data locations. The index is used when searching for data. For all locations you can choose to **Rebuild Index**. This should be done only when a new location is added or if you experience problems while searching (e.g. something is missing from the search results). This operation can take a long time depending on how much data is stored in this location.

If you move the server from one computer to another, you need to move the index as well. Alternatively, you can re-build the index on the new server (this is the default option when you add a location). If the rebuild index operation takes too long and you would prefer to move the

old index, simply copy the folder called `searchindex` from the old server installation folder to the new server.

The status of the index server can be seen in the **User Statistics** pane found in the **Status and Management** tab page showing information on where the index server resides and the number of locations currently being serviced.

3.3 Accessing files on, and writing to, areas of the server filesystem

In various situations, the *CLC Server* needs to read from or write to files on the filesystem outside areas intended for CLC data. Examples include when the data will be imported into the *CLC Server* and when BLAST databases are made available to be searched using functionality of the *CLC Server*. Areas that the *CLC Server* should have read and write access to are configured as **Import/export directories** in the web administrative interface, under the **Main configuration** tab. See figure 3.3.

Note: On grid setups and job node setups, an area configured as import/export directory must be a *shared* directory, accessible from the nodes and from the master server.

Folders configured as import/export directories must be readable and writable by the user that runs the *CLC Server* process. Users logged into the *CLC Server* from their **Import/export directories** can access files in that area, and potentially write files to that area. However, it is the *user running the server process* that actually interacts with the file system.

Permissions can be set on import/export directories, restricting access to certain groups. This is done under the **Global permissions** tab of the web administrative interface.

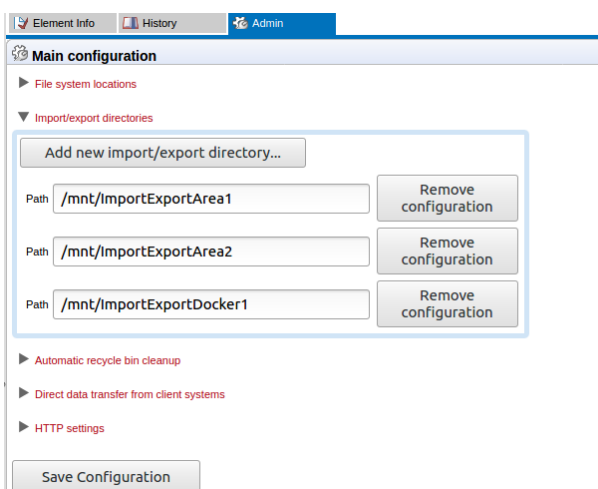


Figure 3.3: *Import/export directories* are configured under the *Main configuration* tab.

Press the **Add new import/export directory** button to enter the relevant path. The specified folder and its subfolders will then be available to *CLC Workbenches* logged into the *CLC Server* when relevant activities, such as import and export, are carried out.

If direct data transfer has been enabled, then *CLC Workbench* users can import data from their local file system to the *CLC Server*. These files are transferred over the network, placed as temporary files in the area configured for this purpose, which will be an import/export directory, and then imported. Direct data transfer configuration is described in section 3.4.

Whether or not direct data transfer has been enabled, they will be able to select file from under areas configured as import/export directories, as illustrated in figure 3.4).

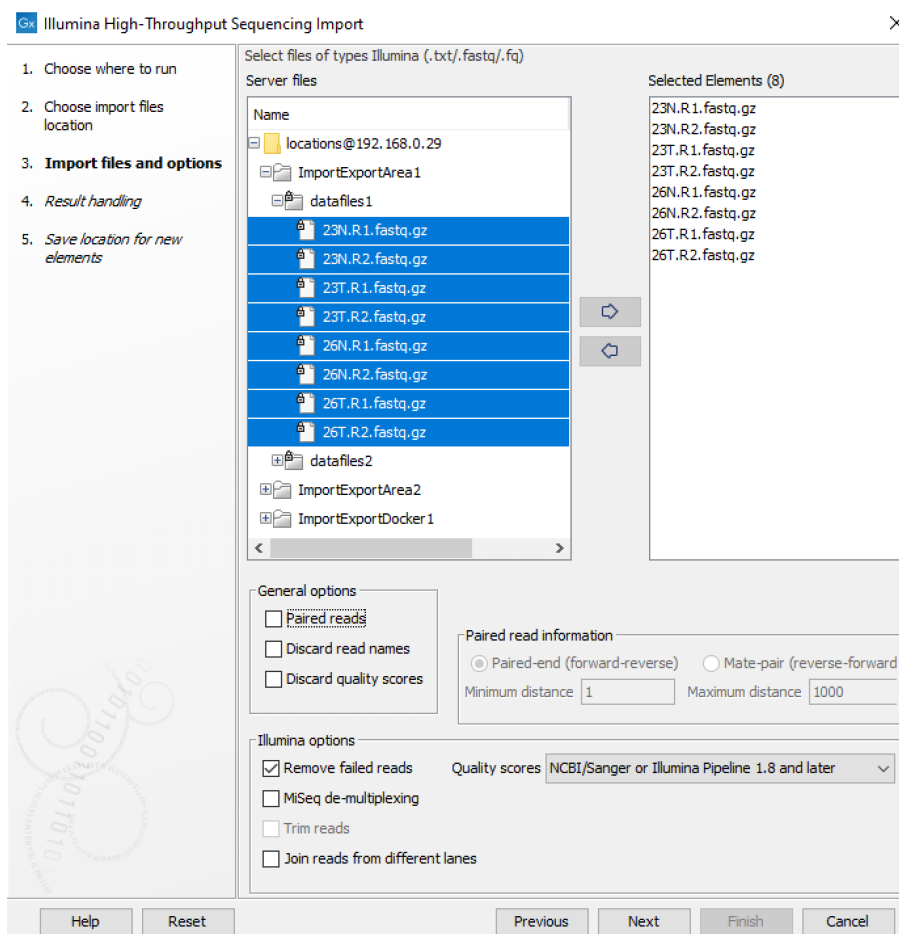


Figure 3.4: A CLC Workbench user can choose to import data using the CLC Server they have logged into and then select files for import that are located in import/export directories.

Note: Import/export directories should NOT be set to subfolders of any defined CLC file or data location. CLC Server file and data locations should be used for data imported into or generated by the CLC software. Import/export directories are intended for holding other data, for example, sequencing data that will be imported, data that is exported from the CLC Server, or BLAST databases.

3.4 Direct data transfer from client systems

By default, transfer of data or files local to client software directly to the CLC Server is not allowed (figure 3.5)¹.

To enable direct data transfer, the option **Files uploaded via Import/Export location** must be selected in the **Direct data transfer from client systems** section under the **Main configuration** tab. For this option to be available to select, at least one import/export directory must be

¹The previous default option, "Files uploaded via temporary file location on server system(s) (legacy)" was removed in CLC Genomics Server 20.0. When upgrading from an earlier version where that option was selected, the new default, "Not allowed" is applied in the updated version.

configured (figure 3.6). If permissions are enabled on the selected import/export directory, the relevant groups must be granted write permission to be allowed to transfer data from their client system to the *CLC Server* directly.

The default setting, "Not allowed", is conservative, and limits certain functionality, including:

- Importing data from a client system (e.g. a system the *CLC Workbench* or *CLC Server Command Line Tools* is on) to a *CLC Server* file system location is not allowed.
- Workflows cannot be installed on the *CLC Server* using the functionality provided by the *CLC Workbench Workflow Manager*.
- Running a standard external application that has parameters referring to files local to a client system is not possible.
- Data cannot be downloaded to a *CLC_References* location on the *CLC Server* via a *CLC Workbench Reference Data Manager*.
- Installing or updating plugins on connected job nodes will fail. (When pushing plugin updates to the nodes, the master is acting as a client to a job node.)

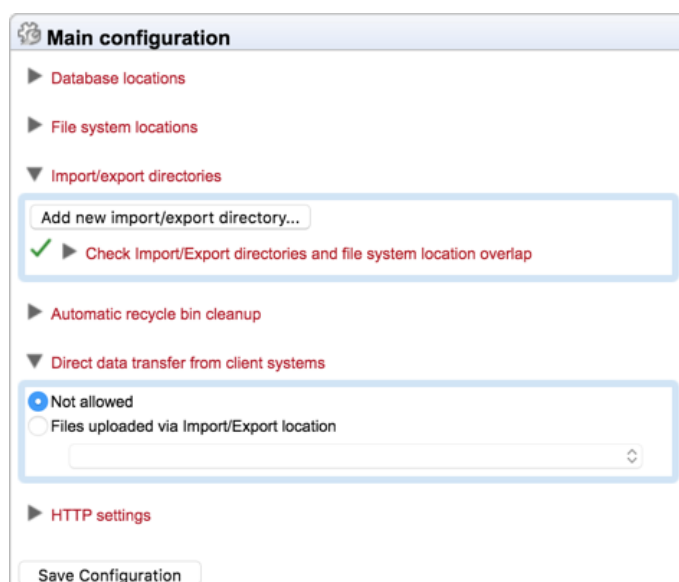


Figure 3.5: By default, transfer of data directly by client software to the *CLC Server* is not allowed. The option allowing such transfers, "Files uploaded via Import/Export location" is disabled if no import/export directory are configured.

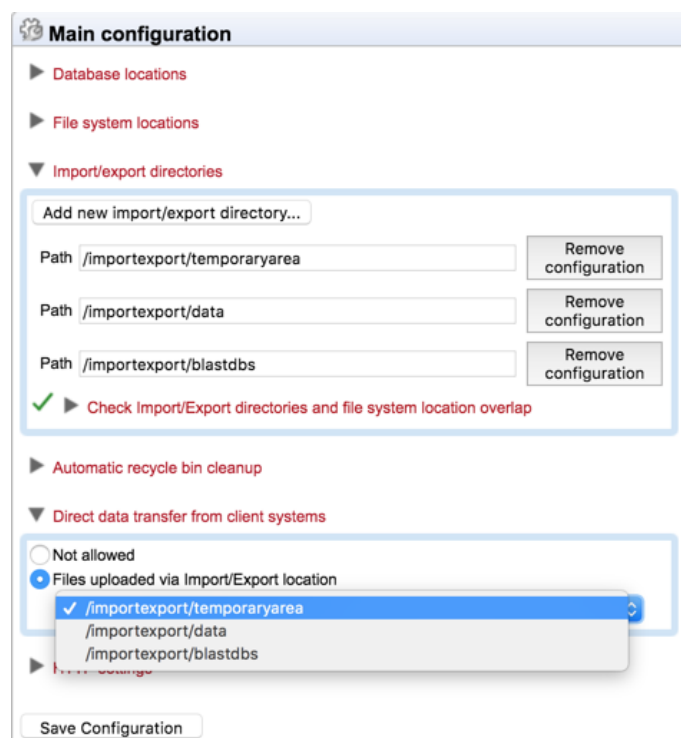


Figure 3.6: An import/export directory must be selected when enabling direct data transfer from client software to the CLC Server.

3.5 Changing the listening port

The default listening port for the CLC Server is 7777. This has been chosen to minimize the risk of collisions with existing web-servers using the more familiar ports 80 and 8080. If you would like to have the server listening on port 80 in order to simplify the URL, this can be done in the following way.

- Navigate to the CLC Server installation directory.
- Locate the file called *server.xml* in the conf directory.
- Open the file in a text editor and locate the following section

```
<Connector port="7777" protocol="HTTP/1.1"
  connectionTimeout="20000"
  redirectPort="8443" />
```

- Change the port value to desired listening port (80 in the example below)

```
<Connector port="80" protocol="HTTP/1.1"
  connectionTimeout="20000"
  redirectPort="8443" />
```

- If you will be using *Genomics Analysis Portal*, create a file named *gap-config.properties* in the CLC Server installation directory. In that file, put the text `server.port=<port>`. For example, for port 80:

```
server.port=80
```

- Restart the service for the changes to take effect. See section 2.7).

- After restarting, log into the web administrative interface and change the default port number in the "Master node port" field under Admin | Job distribution | Server setup, and then click on **Save Configuration** button to save the new setting.

3.6 Changing the tmp directory

The *CLC Server* often uses a lot of disk space for temporary files. These are files needed during an analysis, and they are deleted when no longer needed. By default, these temporary files are written to your system default temporary directory. Due to the amount of space that can be required for temporary files, it can be useful to specify an alternative, larger, disk area where temporary files created by the *CLC Server* can be written.

In the *server installation directory* you will find a file called `CLCServer.vmoptions`, where `CLCServer` will be the name of your particular *CLC server*: `CLCGenomicsServer`

Open the file in a text editor and add a new line like this: `-Djava.io.tmpdir=/path/to/tmp` with the path to the new tmp directory. Restart the server for the change to take effect (see how to restart the server in section 2.7).

We highly recommend that the tmp area is set to a file system local to the server machine. Having tmp set to a file system on a network mounted drive can substantially affect the speed of performance.

3.6.1 Job node setup

The advice about having a tmp area being set on a local file system is true also for job nodes. Here, the tmp areas for nodes should **not** point to a shared folder. Rather, each node should have a tmp area with an identical name and path, but situated on a drive local to each node.

You will need to edit the `CLCServer.vmoptions` file on each job node, as well as the master node, as described above. This setting is **not** pushed out from the master to the job nodes.

3.7 Setting the amount of memory available for the JVM

When running the *CLC Server*, the Java Virtual Machine (JVM) needs to know how much memory it can use. This depends on the amount of physical memory (RAM) and can thus be different from computer to computer. Therefore, the installer investigates the amount of RAM during installation and sets the amount of memory that the JVM can use.

On **Windows** and **Linux**, this value is stored in a property file called `ServerType.vmoptions` (e.g. `CLCGenomicsServer.vmoptions`) which contains a text like this:

```
-Xmx8192m
```

The number (8192) is the amount of memory in megabytes the *CLC Server* is allowed to use. This file is located in the installation folder of the *CLC Server* software.

By default, the value is set to 50% of the available RAM on the system you have installed the software on.

You can manually change the number contained in the relevant line of the `vmoptions` file for your *CLC Server* if you wish to raise or lower the amount of RAM allocated to the Java Virtual Machine.

3.8 Limiting the number of cpus available for use


A number of the algorithms in the *CLC Server* will, in the case of large jobs, use all the cpu available on your system to make the analysis as fast as possible. The maximum number of cpu that can be used can be configured:

Master nodes Configured via the web administrative interface as described in section 6.4².

Job nodes Configured via the web administrative interface as described in section 6.1.

Grid nodes Controlled by the grid scheduler. Further information is available in section 6.3.8.

3.9 HTTP settings

Under the **Admin**  tab, click **Configuration**, and you will be able to specify HTTP settings. Here you can set the time out for the user HTTP session and the maximum upload size (when uploading files through the web interface).

3.10 Deployment of server information to CLC Workbenches

See the *Deployment manual* at <https://digitalinsights.qiagen.com/technical-support/manuals/> for information on pre-configuring the server log-in information when Workbench users log in for the first time.

²The method of using of a `cpu.properties` file to limit CPU usage on master nodes and job nodes is deprecated.

Chapter 4

Managing users and groups

4.1 Logging in the first time and changing the root password

When the server is installed, you will be able to log in via the web interface using the following credentials:

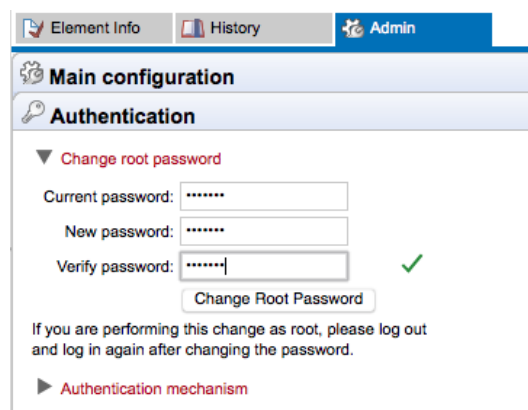
- **User name:** `root`
- **Password:** `default`

Once logged in, you should as a minimum set up user authentication (see section 4.2) and data locations (see section 3.2) before you can start using the server.

For security reasons, you should change the root password (see figure 4.1):

Admin (🔧) | Authentication (🔑) Change root password

Note that if you are going to use job nodes, it makes sense to set these up before changing the authentication mechanism and root password (see section 6).



The screenshot shows a web interface with a navigation bar at the top containing 'Element Info', 'History', and 'Admin'. Below the navigation bar is a 'Main configuration' section with an 'Authentication' sub-section. Under 'Authentication', there is a 'Change root password' section with three password input fields: 'Current password', 'New password', and 'Verify password'. A green checkmark is visible to the right of the 'Verify password' field. Below the input fields is a 'Change Root Password' button. Below the button is a note: 'If you are performing this change as root, please log out and log in again after changing the password.' Below the note is a section for 'Authentication mechanism'.

Figure 4.1: We recommend changing the root password. The verification of the root password is shown with the green checkmark.

4.2 User authentication using the web interface

When the server is installed, you can log in using the default root password (username=root, password=default).

Once logged in, you can specify which of the three modes of authentication should be used by going to:

Admin (⚙️) | Authentication (🔑) Authentication mechanism

The three different modes of authentication are shown in figure 4.2.

If LDAP or Active Directory are selected, a settings panel is revealed, where the details of the integration are specified. An example for LDAP settings is shown in figure 4.3.

Members of a group specified as an administrative group with login rights to the CLC Server will be configure the CLC Server using the functionality under the Admin tab of the web administrative interface, as well as set permissions on folders of data, as described in section 5. For the built-in authentication method, this means adding particular users to the built-in **admin** group. For Active Directory or LDAP, this means designating a group in the box labeled **Admin group name** and adding any users who should be administrators of the CLC Server to this group.

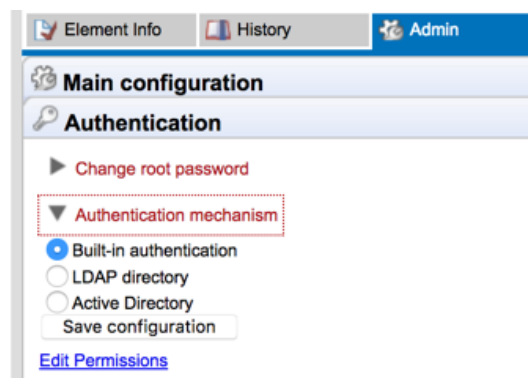


Figure 4.2: Three modes of user authentication are available. Clicking on the [Edit Permissions](#) link at the bottom opens up the [Global Permissions](#) tab, where access to the server and its functionality can be configured, as described in section 5.2.

4.2.1 Authentication options

Built-in authentication

This option will enable you to set up user authentication using the server's built-in user management system. This means that you create users, set passwords, assign users to groups and manage groups using the web interface (see section 4.2.2) or using the Workbench (see section 4.2.4). All the user information is stored on the server and is not accessible from other systems.

LDAP directory

This option will allow you to use an existing LDAP directory. Information needed during authentication and group memberships is then retrieved from that LDAP directory (figure 4.3).

▼ Authentication mechanism

Built-in authentication

LDAP directory

Active Directory

Hostname: host.example.com

Port: 389 Default if "ldaps://" is selected: 636. Else: 389

Encryption: Plain text Default: "Plain text"

Forced Start TLS

ldaps://

Disable SSL certificate check:

Base DN: dc=example,dc=com

Admin group name: admins Default: admins

Cache timeout: 3600 Default: 3600 (seconds)

Users DN: ou=users (Base DN will be appended)

Groups DN: ou=groups (Base DN will be appended)

UID attribute: uid Default: uid

Group name attribute: cn Default: cn

Membership attribute: memberUid Default: memberUid

Bind DN: Leave empty to use anonymous bind for the initial lookup, used to get a user DN

Bind password:

DN to use for lookups:

User DN Select the DN to be used for all search and read operations except for the initial one, for example user and email lookups. The 'DN to use for lookups' option is enabled for selection when Bind DN and password details have been entered above.

Bind DN

User object class: posixAccount

Group object class: posixGroup

Kerberos/GSSAPI Authentication:

Kerberos realm: Leave empty to use default realm

Kerberos config file: /etc/krb5.conf Default: /etc/krb5.conf

Figure 4.3: LDAP settings panel.

Configuration option information

Kerberos/GSSAPI Authentication Enable the LDAP integration to use Kerberos/GSSAPI.

Encryption The default is Plain text, with options available for encryption using Start TLS ("Forced Start TLS") or LDAP over SSL ("ldaps://").

DN to use for lookups This allows you to choose which bind should be used for read and search operations. If no bind DN have been entered an unauthenticated bind will be used to do the initial lookup (lookup of users DN based on the username), and all other read and search operations will be performed with users binds. If the **Bind DN** and **Bind password** have been filled in, you have the choice between using the 'Bind DN' or the 'User DN' for read and search operations, the 'Bind DN' will in this case always be used for the initial lookup.

User object class and Group object class Intended for use where the standard posixAccount and posixGroup classes are not appropriate.

Certificates

If your LDAP server uses a certificate that is not generally trusted by the server system that the CLC Server software is running on, then it must be added to the truststore of the CLC Server

installation (`CLC_SERVER_BASE/jre/lib/security/cacerts`, where `CLC_SERVER_BASE` is the server installations root location). This can be done with the `keytool` shipped with Java installations (also available in the `CLC_SERVER_BASE/jre/bin/keytool`), with a command like:

```
CLC_SERVER_BASE/jre/bin/keytool -import -alias \  
ldap_certificate -file LDAP_CERTIFICATE.cer -keystore \  
CLC_SERVER_BASE/jre/lib/security/cacerts -storepass changeit
```

Replace `LDAP_CERTIFICATE` with the path to the certificate your LDAP server uses for Start TLS/LDAPS connections. Replace `CLC_SERVER_BASE` with the path to the servers installation location.

For a node setup, this must be done for all job nodes as well.

Caution: If you update the server installation or reinstall the server, all imported certificates will be removed, and have to be imported again. You should also be aware that certificates have an expiration date, and will not be trusted after this date. Make sure to add a new certificate in advance of the expiration date.

Active Directory

This option will allow you to use an existing Active directory. This means that all information needed during authentication and group memberships is retrieved from the Active directory. Encryption options (Start TLS and LDAP over SSL) are available. Please see the notes about certificates in the LDAP section (see section 4.2.1) above for details.

4.2.2 Managing users and groups using built-in authentication

This information only applies if built-in authentication is being used.

Managing users via the web administrative interface

To create or remove users or change their password:

Admin (🔑) | Users and groups (👤) Manage user accounts

This will display the panel shown in figure 4.4.

Managing groups via the web administrative interface

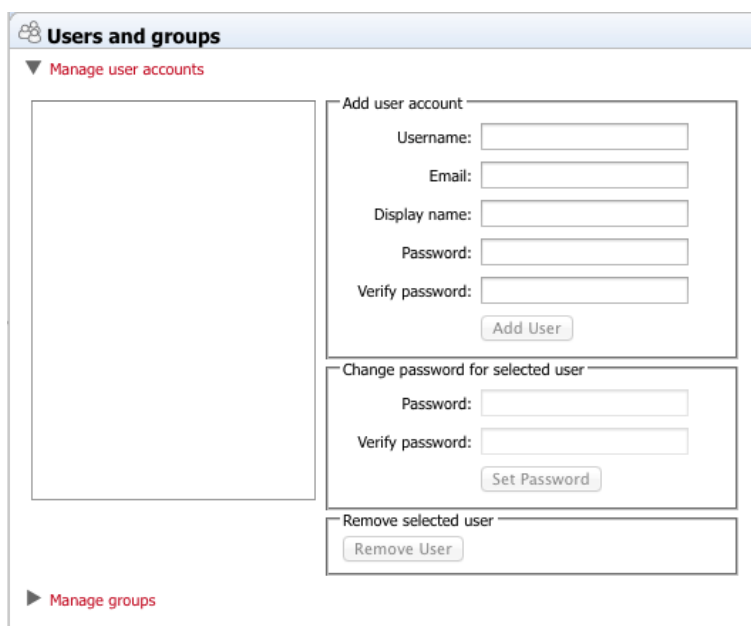
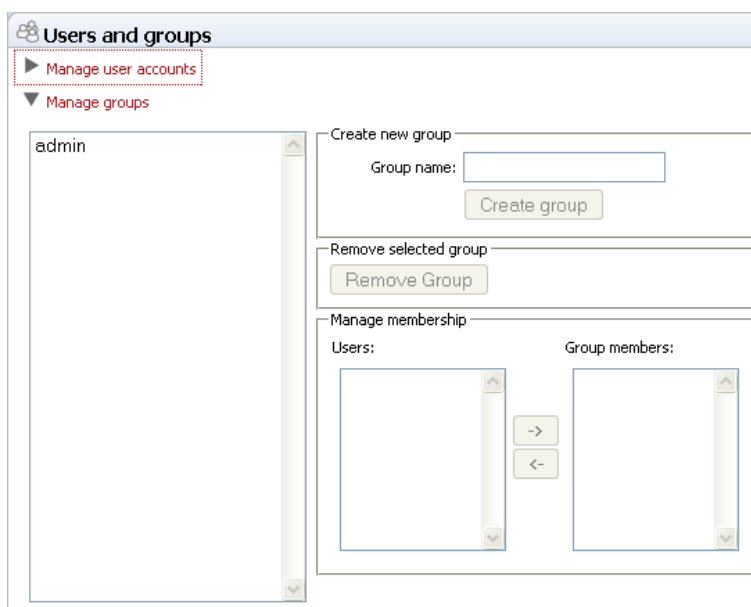
To create or remove groups or change group membership for users when using built-in authentication, go to:

Admin (🔑) | Users and groups (👤) Manage groups

This will display the panel shown in figure 4.5.

The same user can be a member of several groups.

Users who should have access to the administrative part of the server should be part of the "admin" group which is the only group with special permissions by default. The admin group already exists in a default setup of the *CLC Server*.

Figure 4.4: *Managing users.*Figure 4.5: *Managing users.*

You will always be able to log in as the *CLC Server* root user, and this user has administrative level access rights.

4.2.3 User authentication using the Workbench

This information only applies if built-in authentication is being used. If LDAP or AD is being used, the menus described here will be disabled.

Users and groups can be managed through the Workbench by logging into the *CLC Server* as an administrative user and then going to the Workbench menu:

File | Manage Users and Groups

This will display the dialog shown in figure 4.6.

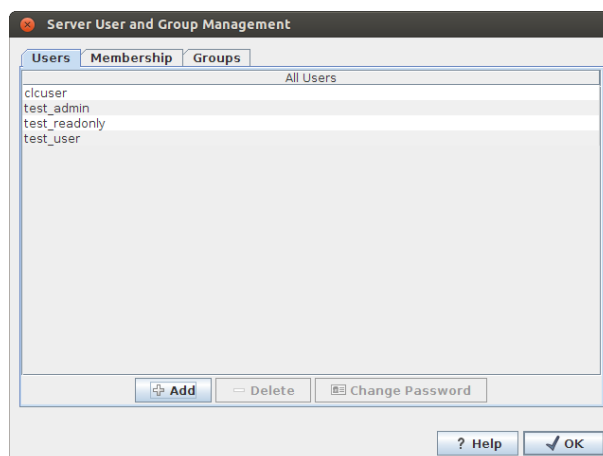


Figure 4.6: Managing users.

4.2.4 Managing users through the Workbench

This information only applies if built-in authentication is being used. If LDAP or AD is being used, the menus described here will be disabled.

Click the **Add** (+) button to create a new user. Enter the name of the user and enter a password. You will be asked to re-type the password. If you wish to change the password at a later time, select the user in the list and click **Change password** (key icon).

To delete a user, select the user in the list and click **Delete** (-).

4.2.5 Managing groups through the Workbench

This information only applies if built-in authentication is being used. If LDAP or AD is being used, the menus described here will be disabled. Access rights are granted to groups, not users, so a user has to be a member of one or more groups to get access to the data location. Here you can see how to add and remove groups, and next you will see how to add users to a group.

Adding and removing groups is done in the **Groups** tab (see figure 4.7).

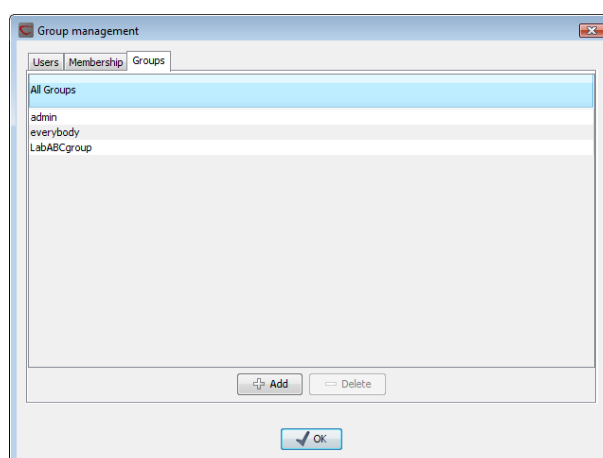


Figure 4.7: Managing groups.

To create a new group, click the **Add** (+) button and enter the name of the group. To delete a group, select the group in the list and click the **Delete** (=) button.

When a new group is created, it is empty. To assign users to a group, click the **Membership** tab. In the **Selected group** box, you can choose among all the groups that have been created. When you select a group, you will see its members in the list below (see figure 4.8). To the left you see a list of all users.

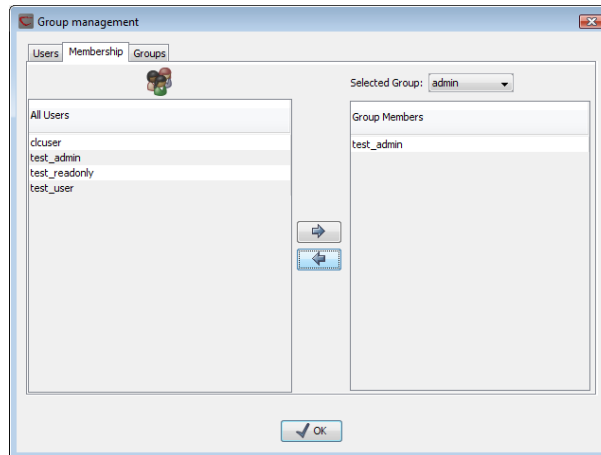


Figure 4.8: Listing members of a group.

To add or remove users from a group, click the **Add** (➡) or **Remove** (⬅) buttons. To create new users, see section 4.2.4.

The same user can be a member of several groups.

Chapter 5

Access privileges and permissions

Server administrators can restrict access to members of specified groups at various levels:

- **Access to the CLC Server**, described in section 5.2.
- **Access to CLC Server data** on file system locations with "Group-based permissions" enabled is described in section 5.1.
- **Launching jobs** on the server, described in section 5.2. This includes setting permissions for data import, data export and for running specified analysis tasks, including built-in analyses, installed workflows and configured External Applications.
- **Access to import/export directories**, described in section 5.2.

5.1 Controlling access to CLC Server data

Folders are the basic unit for controlling access to data. Permissions applied to a folder also apply to the data elements within it. This section describes how to control access to folders on server file locations where permissions have been enabled and the "Group-based permissions" option has been selected, as described in section 3.2.1.

When group-based permissions are enabled on a file system location, initially only the root user or users in a configured admin group have access to data stored there. Permissions are then set by the root user or other admin user on folders using a *CLC Workbench* acting as a client for the *CLC Server*, as described in section 5.1.1.

Members of groups can be granted two types of access:

Read access Members of the designated group(s) can see the elements in the folder, open them and copy from them. Access can be through any client software, for example, via the *CLC Server Command Line Tools* or via a *CLC Workbench*, for example when browsing in the **Navigation Area**, searching, or when clicking the "Originates from" link in the **History** (📄) of a data element.

Write access Members of the designated group(s) can make and **Save** (💾) changes to an element, and new elements and subfolders can be created in that area.

For a user to access a folder, they must have read access to all the folders above it in the hierarchy. In the example shown in figure 5.1, to access the *Sequences* folder, the user must have access to both the *Example Data* and *Protein* folders.

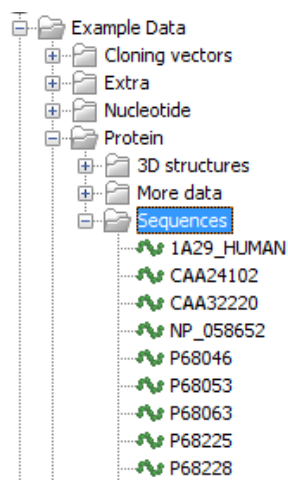


Figure 5.1: A folder hierarchy on the server.

It is fine to just give write access to the final folder. For example, read access only could be granted to the *Example Data* and *Protein* folders, with read and write access granted to the *Sequences* folder.

Please see section 5.1.3 for further details about the system behavior relating to permissions.

5.1.1 Setting permissions on a folder

Setting group-based permissions on a file system location is done using a *CLC Workbench* acting as a client for the *CLC Server*. In the *CLC Workbench*, select the menu option:

File | CLC Server Connection (S)

Log into the *CLC Server* as an administrative user.

You can then set permissions on folders within File Locations that have had group-based permissions enabled, or on Database Locations, if you have the *CLC Bioinformatics Database* extension.

right-click the folder (F) | Permissions (P)

This will open the dialog shown in figure 5.2.

Set the relevant permissions for each of the groups and click **OK**.

If you wish to apply the permissions recursively, that is to all subfolders, check **Apply to all subfolders** in the dialog shown in figure 5.2. **Note** that this operation is usually only relevant if you wish to clean up the permission structure of the subfolders. **It should be applied with caution**, since it can potentially destroy valuable permission settings in the subfolder structure.

5.1.2 Recycle bin

When users delete data in the **Navigation Area** of the Workbench, it is placed in the recycle bin. When the data is situated in a *CLC Server* data location, the data will be placed in a recycle bin

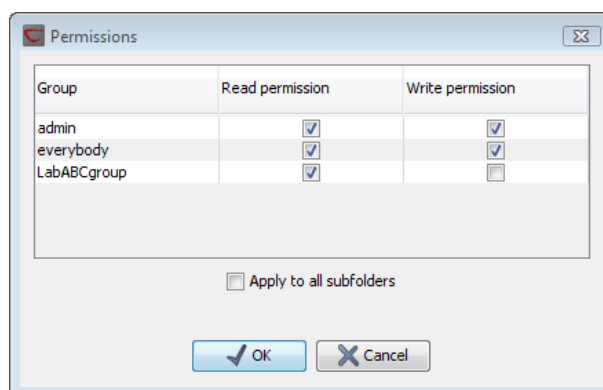


Figure 5.2: Setting permissions on a folder.

for that data location. Each user has an individual recycle bin containing the data deleted by that particular user that cannot be accessed by other users, except server administrators. This means that any permissions applied to the data prior to deletion are no longer in effect, and it is not possible to grant other users permission to see it while it is in the recycle bin. In summary, the recycle bin is a special concept that is not included in the permission control system.

An exception: Deletion of data held in a *CLC Server* file system location named *CLC_References* is different than for other file system locations. Please refer to section 3.2.2 for details.

Server administrators can access the recycle bins of other users through the Workbench:

right-click the data location (📁) | Location | Show All Recycle Bins

This will list all the recycle bins at the bottom of the location as shown in figure 5.3.

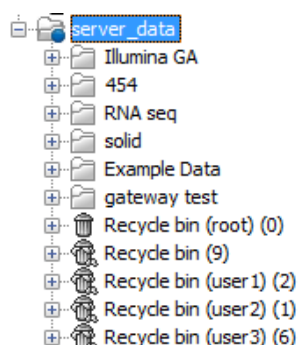


Figure 5.3: Showing all recycle bins.

The recycle bin without a name contains all the data that was deleted in previous versions of the *CLC Server* before the concept of a per-user recycle bin was introduced. This recycle bin can only be accessed by server administrators by selecting **Show All Recycle Bins**.

The administrator is also able to empty the recycle bin of a user:

right-click the recycle bin (🗑️) | Empty

All recycle bins can be emptied in one go:

right-click the data location (📁) | Location | Empty All Recycle Bins

Please note that these operations cannot be undone.

CLC Server can be set to automatically empty recycle bins when the data has been there for

more than 100 days. This behavior can be controlled for each data location: Under the **Main configuration** heading, click the **Automatic recycle bin clean-up** header and click the **Configure** button. This will allow you to disable the automatic clean-up completely or specify when it should be performed as shown in figure 5.4.

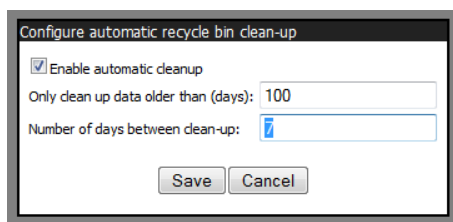


Figure 5.4: Automatic clean-up of the recycle bin.

Data deleted before the per-user recycle bin concept was introduced will be ignored by the automatic clean-up (this is the data located in the general recycle bin that is not labeled with a user name).

5.1.3 Technical notes about permissions and security

All data stored in *CLC Server* file system locations are owned by the user that runs the *CLC Server* process. Changing the ownership of the files using standard system tools is not recommended and will usually lead to serious problems with data indexing and hamper your work on the *CLC Server*.

One implication of the above ownership setup is that without permissions enabled on a file system location, all users logging into the *CLC Server* are able to access all data within that file system location, and write data to that file system locations. All files created within such a file system location are then also accessible to all users of the *CLC Server*.

Group-based and "user homes" permissions on file system locations are additional layers within the *CLC Server*, and are not part of your operating system's permission system. This means that enabling and configuring permissions on server locations only affects users accessing data through *CLC* tools (e.g. using a *CLC Workbench*, the *CLC Server Command Line Tools*, the *CLC Server* web interface or the *Server API*). If users have direct access to the data, using for example general system tools, permissions set on the data via the *CLC Server* has no effect.

In addition, when the "User homes" option is selected for a file system location, any existing group permissions are not applied and data placed directly within the top level folder of that file system location will be readable by any user.

5.2 Controlling access to the server, server tasks and external data

The configurations discussed in this section refer to settings under the **Global Permissions** section of the Admin tab in the *CLC Server* web administrative interface (figure 5.5).

Permissions can be set to restrict access to just the members of specified groups for the following areas:

- **Login restrictions** The ability to log into the *CLC Server*.
- **Algorithms** The analysis algorithms.

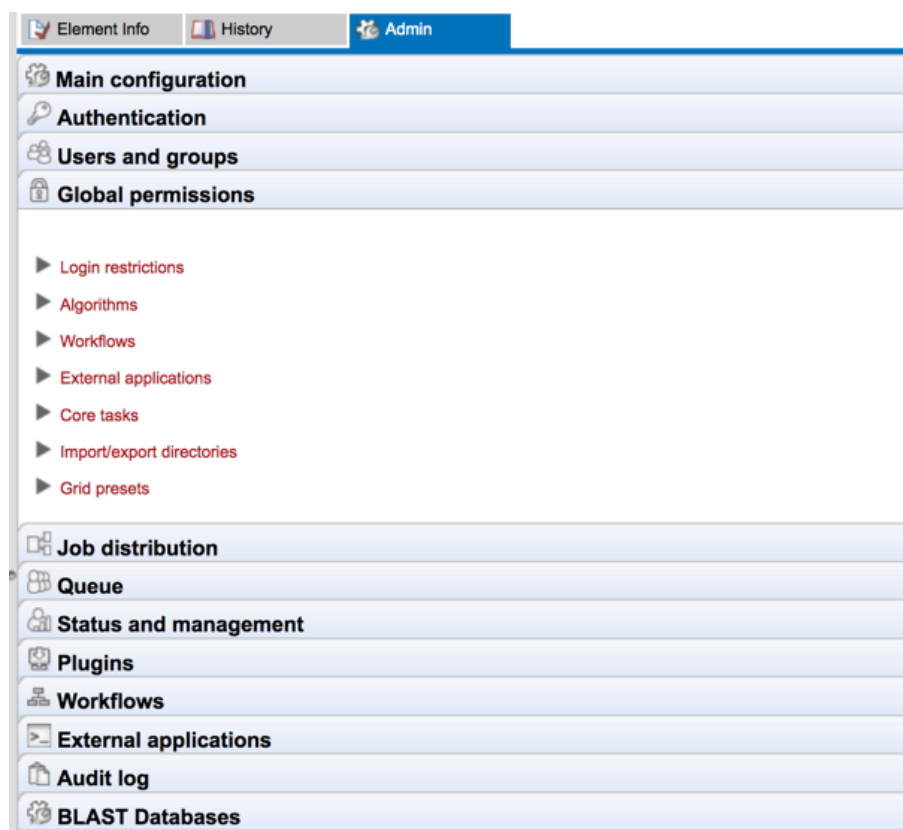


Figure 5.5: *Global permissions*.

- **Workflows** Workflows installed on the server.
- **External applications** External tools configured as External Applications.
- **Core tasks** Currently covers setting permissions on actions associated with the Standard Import tools. (High throughput sequence data import is handled via tools listed in the Algorithms section.)
- **Import/export directories** File system areas not part of the CLC data setup, which the *CLC Server* is able to access. These are described in section 3.3.
- **Grid presets** For grid node setups only: presets for sending jobs to a particular queue with particular parameters. Note that grid presets are identified by name. If you change the name of a preset under the Job Distribution settings section, then this, in effect, creates a new preset. In this situation, if you had access permissions previously set, you would need to reconfigure those settings for this, now new, preset.

You can specify which groups should have access to each of the above by opening the relevant section and then clicking the **Edit Permissions** button for each relevant element listed. A dialog appears like that in figure 5.6. If you choose **Only authorized users from selected groups**, you will be offered a list of groups that you can select (or de-select) to grant or restrict access to that functionality.

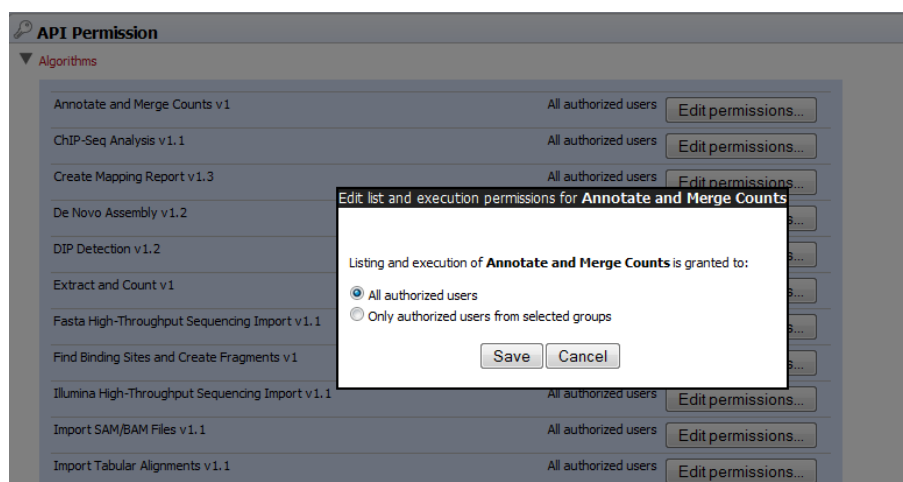


Figure 5.6: Setting permissions for an algorithm.

5.3 Customized attributes on data locations

Location-specific attributes can be set on all elements stored in a given data location. Attributes could be things like company-specific information such as LIMS id, freezer position etc. Attributes are set using a CLC Workbench acting as a client to the CLC Server.

Note that the attributes scheme belongs to a particular data location, so if there are multiple data locations, each will have its own set of attributes.

To configure which fields that should be available¹ go to the Workbench:

right-click the data location | Location | Attribute Manager

This will display the dialog shown in figure 5.7.

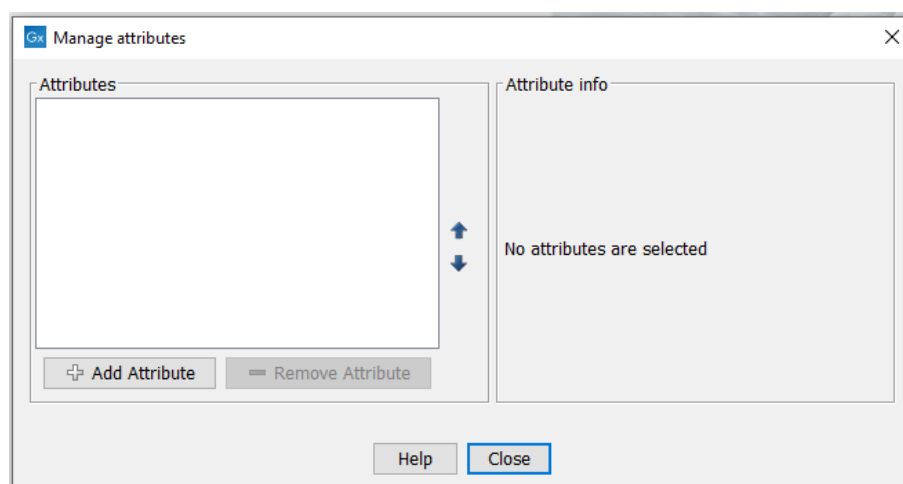


Figure 5.7: Adding attributes.

Click the **Add Attribute** (+) button to create a new attribute. This will display the dialog shown in figure 5.8.

First, select what kind of attribute you wish to create. This affects the type of information that can be entered by the end users, and it also affects the way the data can be searched. The

¹If the data location is a server location, you need to be a server administrator to do this.

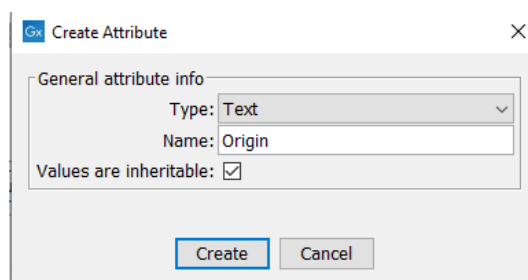


Figure 5.8: The list of attribute types.

following types are available:

- **Checkbox.** This is used for attributes that are binary (e.g. true/false, checked/unchecked and yes/no).
- **Text.** For simple text with no constraints on what can be entered.
- **Hyper Link.** This can be used if the attribute is a reference to a web page. A value of this type will appear to the end user as a hyper link that can be clicked. Note that this attribute can only contain one hyper link. If you need more, you will have to create additional attributes.
- **List.** Lets you define a list of items that can be selected (explained in further detail below).
- **Number.** Any positive or negative integer.
- **Bounded number.** Same as number, but you can define the minimum and maximum values that should be accepted. If you designate some kind of ID to your sequences, you can use the bounded number to define that it should be at least 1 and max 99999 if that is the range of your IDs.
- **Decimal number.** Same as number, but it will also accept decimal numbers.
- **Bounded decimal number.** Same as bounded number, but it will also accept decimal numbers.

When a data element is copied, attribute values are transferred to the copy of the element by default. To prevent the values for an attribute from being copied, uncheck the **Values are inheritable** checkbox.

When you click **OK**, the attribute will appear in the list to the left. Clicking the attribute will allow you to see information on its type in the panel to the right.

Lists are a little special, since you have to define the items in the list. When you choose to add the list attribute in the left side of the dialog, you can define the items of the list in the panel to the right by clicking **Add Item (+)** (see figure 5.9).

Remove items in the list by pressing **Remove Item (−)**.

Removing attributes To remove an attribute, select the attribute in the list and click **Remove Attribute (−)**. This can be done without any further implications if the attribute has just been created, but if you remove an attribute where values have already been given for elements in the

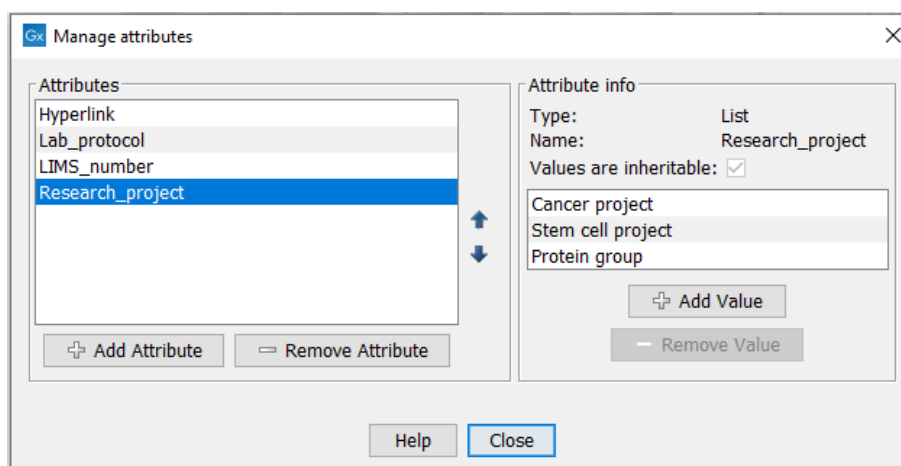


Figure 5.9: Defining items in a list.

data location, it will have implications for these elements: The values will not be removed, but they will become static, which means that they cannot be edited anymore.

If you accidentally removed an attribute and wish to restore it, this can be done by creating a new attribute of exactly the same name and type as the one you removed. All the "static" values will now become editable again.

When you remove an attribute, it will no longer be possible to search for it, even if there is "static" information on elements in the data location.

Renaming and changing the type of an attribute is not possible - you will have to create a new one.

Changing the order of the attributes You can change the order of the attributes by selecting an attribute and click the **Up** and **Down** arrows in the dialog. This will affect the way the attributes are presented for the user.

5.3.1 Filling in values

When a set of attributes has been created (as shown in figure 5.10), the end users can start filling in information.

This is done in the element info view:

right-click a sequence or another element in the Navigation Area | Show (🔍) | Element info (📄)

This will open a view similar to the one shown in figure 5.11.

You can now enter the appropriate information and **Save**. When you have saved the information, you will be able to search for it (see below).

Note that the element (e.g. sequence) needs to be saved in the data location before you can edit the attribute values.

When nobody has entered information, the attribute will have a "Not set" written in red next to the attribute (see figure 5.12).

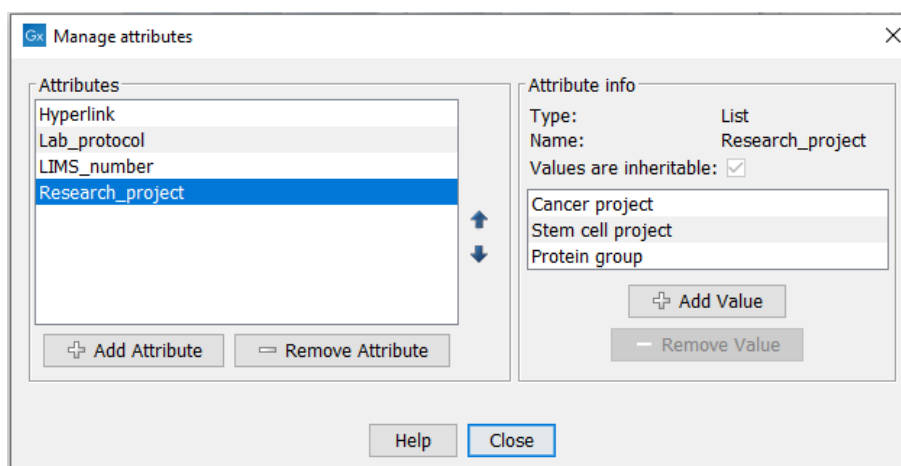


Figure 5.10: A set of attributes defined in the attribute manager.



Figure 5.11: Adding values to the attributes.

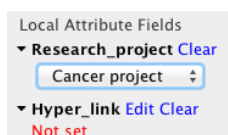


Figure 5.12: An attribute which has not been set.

This is particularly useful for attribute types like checkboxes and lists where you cannot tell, from the displayed value, if it has been set or not. Note that when an attribute has not been set, you cannot search for it, even if it looks like it has a value. In figure 5.12, you will *not* be able to find this sequence if you search for research projects with the value "Cancer project", because it has not been set. To set it, simply click in the list and you will see the red "Not set" disappear.

If you wish to reset the information that has been entered for an attribute, press "Clear" (written in blue next to the attribute). This will return it to the "Not set" state.

The **Folder editor**, invoked by pressing **Show** on a given folder from the context menu, provides a quick way of changing the attributes of many elements in one go (see the Workbench manuals at <https://digitalinsights.qiagen.com/technical-support/manuals/>).

5.3.2 What happens when a clc object is copied to another data location?

The user supplied information, which has been entered in the **Element info**, is attached to the attributes that have been defined in this particular data location. If you copy the sequence to another data location or to a data location containing another attribute set, the information will become fixed, meaning that it is no longer editable and cannot be searched for. Note that attributes that were "Not set" will disappear when you copy data to another location.

If the element (e.g. sequence) is moved back to the original data location, the information will again be editable and searchable.

If the e.g. Molecule Project or Molecule Table is moved back to the original data location, the information will again be editable and searchable.

5.3.3 Searching

When an attribute has been created, it will automatically be available for searching. This means that in the **Local Search** (🔍), you can select the attribute in the list of search criteria (see figure 5.13).

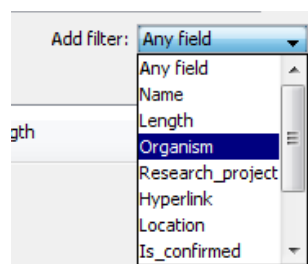


Figure 5.13: The attributes from figure 5.10 are now listed in the search filter.

It will also be available in the **Quick Search** below the **Navigation Area** (press Shift+F1 (Fn+Shift+F1 on Mac) and it will be listed - see figure 5.14).

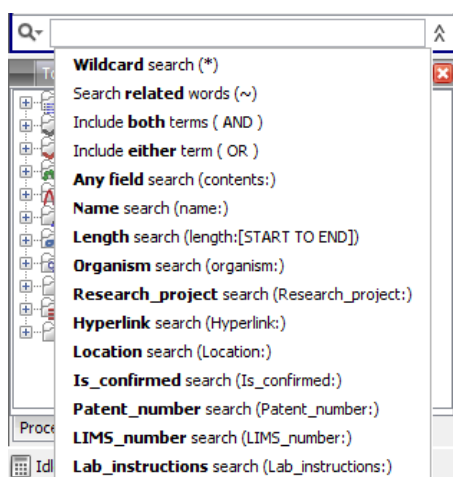


Figure 5.14: The attributes from figure 5.10 are now available in the Quick Search as well.

Read more about search here: http://resources.qiagenbioinformatics.com/manuals/clcgenomicsworkbench/current/index.php?manual=Local_search.html.

Chapter 6

Job distribution

The *CLC Server* has the concept of *distributing jobs to nodes*. This means having a master server with the primary purpose of handling user access, serving data to users and starting jobs, and one or more nodes, which execute the jobs submitted to them. This chapter describes the server setups that are available for the *CLC Server* as well as some job running options available for single servers and those running *CLC* job nodes.

6.1 Introduction to servers setups

The three models for running the *CLC Server* are:

- **Model I: Master server with dedicated job nodes.** In this model, a master server submits *CLC* jobs directly to machines running the *CLC Server* for execution. In this setup, a group of machines (from two upwards) have the *CLC Server* software installed on them. The system administrator assigns one of them as the *master node*. The master controls the queue and distribution of jobs and compute resources. The other nodes are *job nodes*, which execute the computational tasks they are assigned. This model is simple to set up and maintain, with no other software required. However, it is not well suited to situations where the compute resources are shared with other systems because there is no mechanism for managing the load on the computer. This setup works best when the execute nodes are machines dedicated to running a *CLC Server*. Further details about this setup can be found in section [6.1](#)
- **Model II: Master server submitting to grid nodes.** In this model, a master server submits tasks to a local third party scheduler. That scheduler controls the resources on a local computer cluster (grid) where the job will be executed. This means that it is the responsibility of the native grid job scheduling system to start the job. When the job is started on one of the grid nodes, a **CLC Grid Worker**, which is a stand-alone executable including all the algorithms on the server, is started with a set of parameters specified by the user. Further details about this setup can be found in section [6.3](#).
- **Model III: Single Server setup.** In this model, the master and execution node functionality is carried out by a single *CLC Server* instance.

Figure [6.1](#) shows a schematic overview.

For models I and II, the master server and job nodes, or master server and grid nodes must run on the same type of operating system. It is not possible to have a master server running Linux and a job node running Windows, for example.

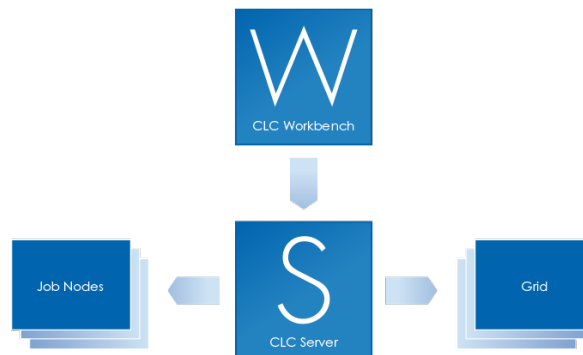


Figure 6.1: An overview of the job distribution possibilities.

6.2 Model I: Master server with dedicated job nodes

6.2.1 Overview: Model I

This setup consists of two types of CLC Server instances:

1. **A master node** - a machine that accepts jobs from users and then passes them to job nodes for execution.
2. **Job nodes** - machines running the *CLC Server* that accept jobs directly from a master node.

The general steps for setting up this model are:

1. Install the *CLC Server* software on all the machines involved. (See section 2.2.)
2. Install the license on the machine that will act as the master node. (See section 2.6.)
3. Start up the *CLC Server* software on the master server. Then start up the software on the job nodes. (See section 2.7.)
4. Log in to the web administrative interface for the *CLC Server* of the master node. (See section 9.)
5. Configure the master node, attach the job nodes and configure the job nodes via the administrative interface on the master node.

Almost all configuration for the CLC Server cluster is done via the web administrative interface for the *CLC Server* on the **master node**. This includes the installation of plugins. See section 6.2.3.

The only work done directly on the machines that will run as job nodes is

- Installation of the *CLC Server* software.
- Starting up the software up on each node.

- The changing of the built-in administrative login credentials under certain circumstances. See section 6.2.1.
- If using a CLC Bioinformatics Database, installing the relevant database driver on each job node.

6.2.2 User credentials on a master-job node setup

When initially installed, all instances of the *CLC Server* will have the default admin user credentials.

If you have a brand new installation, and you are happy to use the default administrative login credentials (see section 9) during initial setup, you do not need to change anything.

Once the *CLC Server* software on all machines is up and running and the job nodes have been attached to the master, changes to passwords for the built-in authentication system, which includes the default admin user, root, will be pushed from the master to the job nodes. You do not need to manually change the password on each job node.

If you wish to change the default administrative password before attaching the job nodes to the master, then please log into the web administrative interface of each machine running the *CLC Server* software and setup *identical* details on each one.

The master node needs access to the job nodes to be able to push configurations to them. Thus, if you change the admin password on the master server and later wish to attach a new job node, you will need to log into the web administrative interface of the job node and set the root password for the *CLC Server* software to match that of the master server. Until that is done, the master will not be able to communicate with the job node because the root admin passwords are different. Once the master can communicate with the job node, it can push other configurations to the job node.

6.2.3 Configuring your setup

If you have not already, please download and install your license to the master node. (See section 2.6.) Do **not** install license files on the job nodes. The licensing information, including how many job nodes you can run, are all included in the license on the master node.

To configure your master/execution node setup, go to the Job distribution tab in the web administrative interface on the master node:

Admin (⚙️) | **Job distribution** (📄)

Then enter the following information:

- **Server mode** - select `MASTER_NODE`.
- **Master node host** - Enter the master node host name. Click on the "Show suggestions" text next to this field to see information about the server that can be useful when configuring this option.
- **Master node port** - usually `7777`
- **Master node display name** - the name shown in the top bar of the web interface for the *CLC Server*

- **CPU limit** - The maximum number of CPU the CLC Server should use. This is set to unlimited by default, meaning that up to all cores of the system can be used.

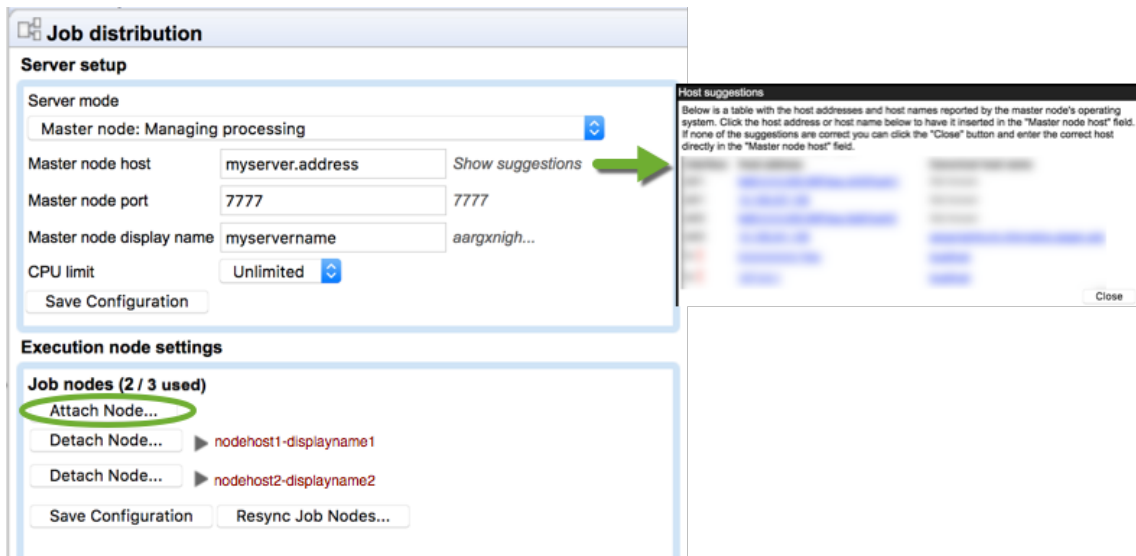


Figure 6.2: Setting up a master server.

Click on the button **Save Configuration** to register the changes just made.

If the **Attach Node** button in the Job nodes section is greyed out, please ensure that the server mode selected is `MASTER_NODE` and that you have clicked on the **Save Configuration** button to save your configuration changes.

Then, for each job node:

- Click on the **Attach Node** button to specify a job node to attach. See figure 6.2.
- Enter information about the node in the fields (see figure 6.3).

Figure 6.3: Add new job node.

- Optionally, click on the button labeled "Manage Job Types" to specify the types of jobs that can be run on each node. See figure 6.4. The default is "Any installed Server Command". If you choose instead "Only selected Server Commands", a search field and a list of all server command names and types will appear. The search field can be used to narrow down the server commands by name or type. Only the tools selected can then be run on that particular job node. Click **Modify** when you are done.

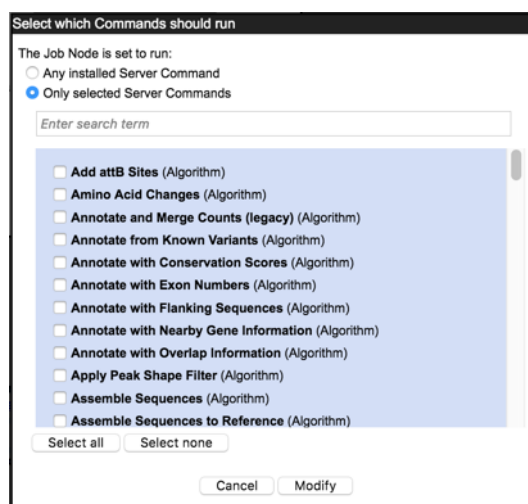


Figure 6.4: Select Server Commands to run on the job node.

- Click **Create**.

Repeat this process for each job node you wish to attach and click **Save Configuration** when you are done.

You will get a warning dialog if there are types of jobs that are not enabled on any of the nodes.

Note that when a node has finished a job, it will take the first job in the queue that is of a type the node is configured to process. This then means that, depending on how you have configured your system, the job that is number one in the queue will not necessarily be processed first.

To test that access works for both job nodes and the master node, you can click "check setup" in the upper right corner as described in section 15.1.

One relatively common problem that can arise is *root squashing*. This often needs to be disabled, because it prevents the servers from writing and accessing the files as the same user - read more about this at http://nfs.sourceforge.net/#faq_b11.

Once set up, job nodes automatically inherit all configurations on the master node. If one of the job nodes gets out of sync with the master, click the **Resync job nodes** button, shown in figure 6.2. This should not be done while jobs are running on any nodes. The server can be put into Maintenance Mode to allow current jobs to complete before maintenance tasks are carried out. See section 7.3.

6.2.4 Installing Server plugins on job nodes

You **only** need to install or uninstall plugins on the master server. The *CLC Server* master and all job nodes need to be restarted to complete the installation or removal of plugins. This is easily accomplished by using the **Restart** option in the **Server Maintenance** section under the **Status and management** area on the master server, which restarts the master and all the job nodes. See section 7.

Server plugin installation and removal is described in section 10.

Once a plugin is installed, you should **check that the plugin is enabled** for **each job node** you wish to make available for users to run that particular task on. To do this:

- Go to the Job Distribution tab in the master nodes web administrative interface
- Click on the link to each job node
- Click in the box by the relevant task, marking it with a check mark if you wish to enable it.

6.3 Model II: Master server submitting to grid nodes

6.3.1 Overview: Model II

The CLC Grid Integration allows jobs to be offloaded from a master server onto grid nodes using the local grid submission/queuing software to handle job scheduling and submission.

A given CLC algorithm will only run on a single machine, i.e., a single job will run on one node. Each grid node employed for a given task must have enough memory and space to carry out that entire task.

The grid system uses two locations for its deployment:

- **Path to CLC Grid Worker** in the grid preset editor. This location is used for plugins, a grid version of the server, i.e., the code that is executed when a grid job is started, licences, libraries and more. Grid workers are redeployed in two situations: 1) When the server starts up and 2) If the configuration of one of the grid presets is changed, in which case the grid workers of all presets are redeployed. In addition, the grid workers are updated when a plugin is installed or removed.
- **Shared work directory.** This location is where each grid job gets its own sub directory in which it places its temporary data, e.g., the description of the job to be executed, the configurations files that the grid version of the server needs in order to setup persistence models and log files. This location is only deployed once, either when the grid job starts executing (in case of workflow jobs) or when the grid job is queued (in all other cases).

6.3.2 Requirements for CLC Grid Integration

- A functional grid submission system must already be in place. Please also see the section on supported job submission systems below.
- The DRMAA library for the grid submission system to be used. See Appendix section [17.5](#) for more information about DRMAA libraries for the supported grid submission systems.
- The *CLC Server* must be installed on a Linux based system configured as a *submit host* in the grid environment.
- The user running the *CLC Server* process is seen as the submitter of the grid job, and thus this user must exist on all the grid nodes.
- *CLC Server* file locations holding data that will be used must be mounted with the same path on the grid nodes as on the master *CLC Server* and accessible to the user that runs the *CLC Server* process.
- If a *CLC Bioinformatics Database* is in use, all the grid nodes must be able to access that database using the user that runs the *CLC Server* process.

- A *CLC Network License Manager* with one or more available *CLC Grid Worker* licenses must be reachable from the *execution hosts* in the grid setup.

Supported grid scheduling systems

Grid integration in CLC Genomics Server is done using DRMAA, described further in the appendix 17.5. We have verified grid integration functionality using the following third party scheduling systems:

- SLURM 16.05.2
- UNIVA 8.4.1
- LSF 9.1.1 and 10.1
- PBS Pro 14.2.1

Integration using other grid scheduling systems is anticipated to work as long there is a working DRMAA library and a mechanism to limit the number of CLC jobs launched for execution such that when this number exceeds the number of CLC Grid Worker licenses, excess tasks are held in the queue until a license becomes available.

For SLURM, the number of CLC Grid Worker licenses can be configured as described on <https://slurm.schedmd.com/licenses.html>. For LSF and UNIVA, a "Consumable Resource" would be configured, as described in section 6.3.6. Relevant information about configuring consumable resources for PBS Pro can be found in the administrator's guide for that scheduling software.

TORQUE from Adaptive Computing is an example of a system that works for submitting CLC jobs, but that cannot be supported because it does not provide a means of limiting the number of CLC jobs. As far as we know, there is no way to limit the number of CLC jobs sent simultaneously to the cluster to match the number of CLC Grid Worker licenses. So, with TORQUE, if you had three Grid Worker licenses, up to three jobs could be run simultaneously. However, if three jobs are already running and you launch a fourth job, then this fourth job will fail because there would be no license available for it. This limitation can be overcome, allowing you to work with systems such as TORQUE, if you control the job submission in some other way so the license number is not exceeded. One possible setup for this is if you have a one-node-runs-one-job setup. You could then set up a queue where jobs are only sent to a certain number of nodes, where that number matches the number of CLC Grid Worker licenses you have.

6.3.3 Technical overview

Figure 6.5 shows an overview of the communication involved in running a job on the grid, using OGE as the example submission system.

The steps of this figure are in detail:

1. From the Workbench the user invokes an algorithm to be run on the grid. This information is sent to the master server running the *CLC Server*.

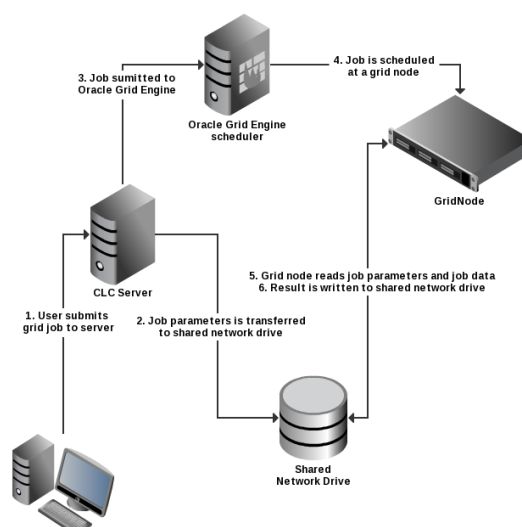


Figure 6.5: An overview of grid integration, using OGE as the example submission system.

2. The master server writes a file with job parameters to a shared work directory of the grid execution nodes. The job parameters contain identifiers mapping to the job data placed in the CLC server data location. The job parameters file is automatically deleted when it is no longer used by the grid node.
3. Now the server invokes *qsub* through the specified DRMAA native library. Then *qsub* transfers the job request to the grid scheduler. Since the user that runs the CLC Server process has invoked *qsub*, the grid node will run the job as this CLC-Server user.
4. The job scheduler will choose a grid node based on the parameters given to *qsub* and the user that invoked *qsub*.
5. The chosen grid node will retrieve CLC Grid Worker executable and the job parameters from the shared file system and start performing the given task.
6. After completion of the job, the grid node will write the results to the server's data location. After this step the result can be accessed by the Workbench user through the master server.

6.3.4 Setting up the grid integration

CLC jobs are submitted to a local grid via a special, stand-alone executable called **clcgridworker**. In the documentation, this executable is also referred to as the CLC Grid Worker.

The following steps are taken to setup grid integration for CLC jobs. These steps are described in more detail in the sections that follow. It is assumed that your *CLC Server* software is already installed on the machine that is to act as the master.

1. Set up the licensing of the grid workers, as described in section [6.3.5](#)
2. Configure the CLC grid licenses as a consumable resource in the local grid system, as described in section [6.3.6](#)
3. Configure and save grid presets, as described in section [6.3.7](#)

4. Optionally, create and edit a `clcgridworker.vmoptions` file in each deployed CLC Grid Worker area, as described in section 6.3.10.
5. Test your setup by submitting some small tasks to the grid via a CLC Server client, such as a CLC Genomics Workbench or the CLC Server Command Line Tools. Ideally, these would be tasks already known to run smoothly directly on your CLC Server.

6.3.5 Licensing of grid workers

There are two main steps involved in setting up the licenses for your CLC Grid Workers.

Step 1: Installing network licenses and making them available for use

Generally, a pool of CLC grid licenses are purchased and are served by the *CLC Network License Manager* software. For information on how to install the *CLC Network License Manager* and download and install your CLC Grid Worker licenses please follow the instructions in the *CLC Network License Manager* user manual, which can be found at

<https://resources.qiagenbioinformatics.com/manuals/clclicensesserver/current/>.

A pdf version is available at

https://resources.qiagenbioinformatics.com/manuals/clclicensesserver/current/User_Manual.pdf.

Step 2: Configuring the location of your CLC License Server for your CLC Grid Workers

One license is used for each CLC Grid Worker script launched. When the CLC Grid Worker starts running on a node, it will attempt to get a license from the license server. Once the job is complete, the license will be returned. Thus, your CLC Grid Worker needs to know where it can contact your CLC License Server to request a license.

To configure this, use a text editor and open the file: `gridres/settings/license.properties` under the installation area of your CLC Server.

The file will look something like this:

```
#License Settings

serverip=host.example.com
serverport=6200
disableborrow=false

autodiscover=false
useserver=true
```

You can leave `autodiscover=true` to use UDP-based auto discovery of the license server. However, for grid usage it is recommended that you set `autodiscover=false` and use the `serverip` property to specify the host name or IP-address of your CLC License Server.

After you have configured your grid presets, see section 6.3.7, and have saved them, those presets are deployed to the location you specify in the **Path to CLC Grid Worker** field of the preset. Along with the `clcgridworker` script, the license settings file is also deployed.

If you need to change your license settings, we recommend that you edit the `license.properties` file under `gridres/settings/license.properties` of your *CLC Server* installation, and then re-save each of your grid presets. This will re-deploy the CLC Grid Workers, including the changed `license.properties` file.

6.3.6 Configuring licenses as a consumable resource

Since there is a limitation on the number of licenses available, it is important that the local grid system is configured so that the number of CLC Grid Worker scripts launched is never higher than the maximum number of licenses installed. If the number of CLC Grid Worker scripts launched exceeds the number of licenses available, jobs unable to find a license will fail when they are executed.

Some grid systems support the concept of a *consumable resource*. Using this, you can set the number of CLC grid licenses available. This will restrict the number of CLC jobs launched to run on the grid at any one time to this number. Any job that is submitted while all licenses are already in use should sit in the queue until a license becomes available. **We highly recommend that CLC grid licenses are configured as a consumable resource on the local grid submission system.**

Information about how a consumable resource can be configured for LSF has been provided by IBM and can be found in Appendix section [17.6](#)

6.3.7 Configure grid presets

A **grid preset** contains information needed for jobs to be handled by the *CLC Server* and submitted to the grid scheduling system. Multiple grid presets can be configured. Users specify the relevant grid preset when submitting a job. See also section [6.3.12](#).

To configure a grid preset, log into the web interface of the *CLC Server* master and navigate to:

Admin (⚙️) | **Job distribution** (📁)

In the **Grid setup** section, under **Grid Presets**, click on the **Create New Preset** button.

Create new grid preset	
Preset name	Example Preset 1
Native library path	/usr/lib/libdrmaa.so
Shared work directory	/mnt/shared/tmp/gridworker
Path to CLC Grid Worker	/mnt/shared/gridworker/clcgridworker
Job category	
CLC Grid Worker memory limit	10g
Grid Mode	<input type="radio"/> Legacy <input checked="" type="radio"/> Resource Aware
Native specification f(x)...	
Submit test job...	
Shared native specification f(x)...	-n {COMMAND_THREAD_MIN},{COMMAND_THREAD_MAX}
Submit test job...	
<input type="button" value="Cancel"/> <input type="button" value="Save Configuration"/>	

Figure 6.6: The grid preset configuration form. The Shared native specification field is only visible when the Resource Aware grid mode is selected.

Preset name The preset name will be specified by users when submitting a job to the grid. See

section 6.3.12). Preset names can contain alphanumeric characters and hyphens. Hyphens cannot be used at the start of preset names.

Native library path The full path to the grid-specific DRMAA library.

Shared work directory The path to a directory that can be accessed by both the CLC Server and the Grid Workers. Temporary directories are created within this area during each job run to hold files used for communication between the CLC Server and Grid Worker.

Path to CLC Grid Worker The path to a directory on a shared file system that is readable from all execution hosts. If this directory does not exist, it will be created.

The CLC Grid Worker and associated settings files are extracted from the installation area of the *CLC Server* software and are deployed to this location when the grid preset is saved and whenever plugins are updated on the *CLC Server*¹.

Job category The name of the job category - a parameter passed to the underlying grid system.

CLC Grid Worker memory limit The maximum amount of memory the CLC Grid Worker java process should use. This field is useful if the memory limit set by auto-detection is not appropriate. The value is given as a number followed by a unit, 'g', 'm' or 'k' for gigabytes, megabytes or kilobytes respectively. For example, "10g" would limit the CLC Grid Worker java process to using a maximum of 10 GB of memory. If left blank, auto-detection is used to determine the limit. See section 6.3.14 for further details.

Grid mode There are two grid modes for backwards compatibility reasons. The "Resource Aware" mode is generally recommended. Choosing this mode allows jobs that require few resources to run concurrently on a given node. For this, the field **Shared native specification** must also be configured. This is described further below. If "Legacy mode" is selected, all jobs submitted to the grid from the *CLC Server* will request use of the entire node. "Legacy Mode" is the default, but this may change in the future.

Native specification and Shared native specification Parameters to be passed to the grid scheduler are specified here. For example, a specific grid queue or limits on numbers of cores. Clicking on the f(x) next to the field name pops up a box containing the variables that will be evaluated at run time. These are described further below.

The **Native specification** field contains the information to be passed to the grid scheduler for exclusive jobs, those where the whole execution node will be used.

The **Shared native specification** contains the information to be passed to the grid scheduler for jobs classified as non-exclusive. Such jobs can share the execution node with other jobs. This specification is only visible and configurable if the "Resource Aware" grid mode is selected.

Exclusive, streaming and non-exclusive tasks are described in section 6.8.1 and further configuration for running concurrent jobs is described in the section on Multi job processing on grid 6.3.9

¹In versions of *CLC Server* earlier than 5.0, this path needed to point at the *clcgridworker* script itself.

<i>Grid mode</i>	Exclusive Jobs	Non-exclusive jobs
<i>Legacy</i>	Native specification	NA - all jobs treated as exclusive
<i>Resource aware</i>	Native specification	Shared native specification

Table 6.1: Summary of grid modes and the specifications used for exclusive jobs, requiring a whole node, and non-exclusive jobs, which can share a node with other jobs.

Below are examples of OGE-specific arguments one could provide in the native specification field of a grid preset. Please refer to your grid scheduler documentation for information on the options available for your grid system.

Example 1: To redirect standard output and error output, this in a native specification field:

```
-o <path/to/standard_out> -e <path/to/error_out>
```

would result in the following *qsub* command being generated:

```
qsub my_script -o <path/to/standard_out> -e <path/to/error_out>
```

Example 2: To use a specific OGE queue for all jobs, this in a native specification field:

```
-hard -l qname=<name_of_queue>
```

would lead to the following *qsub* command:

```
qsub my_script -q queue_name
```

f(x) - adding variables to be evaluated at run-time

Grid Presets are essentially static in nature, with most options being defined directly in the preset itself. There are, however, 5 variables that can be specified that will be evaluated at runtime.

To aid with the required syntax, click on the *f(x)* link and choose the variable to insert. The variables can also be entered directly into the specification by typing the variable name between a pair of curly brackets.

The available variables are:

USER_NAME The name of the user who submitted the job. This variable might be added to log usage statistics or to send an email to an address that includes the contents of this variable. For example, something like the following could be put into a native specification field:

```
-M {USER_NAME}@yourmailserver.com
```

COMMAND_NAME The name of the *CLC Server* command to be executed on the grid by the *clcgridworker* executable. One example of the use of this variable is to specify `-q {COMMAND_NAME}` if there were certain commands to be submitted to queues of the same name as the command.

COMMAND_ID The ID of the *CLC Server* command to be executed on the grid.

COMMAND_THREAD_MIN A value passed by non-exclusive jobs indicating the minimum number of threads required to run the command being submitted. This variable is only valid for Shared native specifications.

COMMAND_THREAD_MAX A value passed by non-exclusive jobs indicating the maximum number of threads supported by the command being submitted. This variable is only valid for Shared native specifications.

Using functions in native specifications

Two functions can be used in native specifications `take_lower_of` and `take_higher_of`. These are invoked with the syntax: `{#function arg1, arg2, [... argn]}`: These functions are anticipated to be primarily of use in Shared native specifications when limiting the number of threads or cores that could be used by a non-exclusive job, and where the grid system requires a fixed number to be specified, rather than a range.

take_lower_of Evaluates to the lowest integer value of its argument.

take_higher_of Evaluates to the highest integer-value of its argument.

In both cases, the allowable arguments are integers or variable names. If an argument provided is a string that is not a variable name, or if the variable expands to a non-integer, the argument is ignored. For instance `{#take_lower_of 8,4,FOO}` evaluates to 4 and ignores the non-integer, non-variable "FOO" string. Similarly, `{#take_higher_of 8,4,FOO}` evaluates to 8 and ignores the non-integer, non-variable "FOO" string.

An example of use of the `take_lower_of` function in the context of running concurrent jobs on a given grid node is provided in section [6.3.9](#).

6.3.8 Controlling the number of cores utilized

This section covers basics related to setting limits on core or thread usage via a *CLC Server* grid preset. Parameter details are specific to the grid scheduler being used. We provide some information below for some schedulers, but please refer to the grid scheduler documentation for full details.

When using "Legacy mode" grid mode, or when running exclusive jobs with the "Resource Aware" grid mode, the default for all jobs is to assume they have access to all cores on the node they are run on. Details about grid modes can be found in section [6.3.7](#).

When configuring a core or thread limit for exclusive jobs, i.e. those that will require use of a whole node, the relevant parameter(s) and integer value(s) to be used by the grid scheduler are entered directly in the Native specification field. To specify different core limits for different types of tasks, one could set up multiple presets with different values supplied in the Native specification field of each.

Configuration of core requirements is central to supporting concurrent execution of non-exclusive jobs on a grid node. This is done by specifying core or thread requirements in the Shared native specification, making use of the variables `COMMAND_THREAD_MIN`, `COMMAND_THREAD_MAX`

and optionally the functions `take_lower_of` and `take_higher_of`. Further information about this is provided in section [6.3.9](#).

Configuration of OGE

1) CPU Core usage when not using parallel environment

In the *CLC Server*, there is an environmental variable, which when set to 1, specifies that the number of allocated slots should be interpreted as the maximum number of cores a job should be run on. To set this environmental variable, add the following to the Native specification of the grid preset:

```
-v CLC_USE_OGE_SLOTS_AS_CORES=1
```

In this case, the maximum number of cores the job should use will be set to the number of slots allocated by OGE for the job.

2) Limiting CPU core usage when using the parallel environment feature

The parallel environment feature can be used to limit the number of cores used by the *CLC Server* jobs when running on the grid. When the parallel environments feature is used, the number of allocated slots is interpreted as the maximum number of cores to be used by the job. The parallel environment must be setup by the grid administrator in such a way that the number of slots corresponds to the number of cores.

The syntax in the Native specification for using parallel environments is:

```
-pe <pe-name> <min-cores>-<max-cores>
```

where *pe-name* is the name of the parallel environment, and a range of cores is specified with integers, e.g. 1-4.

An example as might be entered into a Native specification when using parallel environments is:

```
-l cfl=1 -l qname=64bit -pe clc 1-3.
```

Here, the *clc* parallel environment is selected and 1 to 3 cores are requested.

Configuration of PBS Pro

With PBS Pro the number of cores to use is specified with a single number. This request can be granted (the process is scheduled) or denied (the process is not scheduled). The number of cores are requested as a resource: `-l nodes=1:ppn=X`, where *X* is the number of cores. Please ensure that *the number of nodes requested is 1*.

An example as might be entered into a Native specification is: `-q bit64 -l nodes=1:ppn=2`. This would request 2 cores and the job would be put in the *bit64* queue.

Configuration of LSF

With LSF the number of cores to use is specified with the `-n` option. This parameter can accept a single argument or two arguments. A single argument, `-n X`, is a request for exactly *X* cores. Two arguments, `-n X, Y`, (separated by a comma), is a request for between *X* and *Y* cores.

6.3.9 Multi-job processing on grid

Certain types of CLC Server jobs, known as "non-exclusive" jobs, can be scheduled to run concurrently on the same grid node when appropriate. Non-exclusive jobs are those that have reasonably low demands for system resources. A list of such jobs is provided in the Appendix, section 17.4.

There are two ways non-exclusive jobs can be configured to run concurrently on a grid node:

1. In the context of a workflow or workflow block executed on a single grid node

If the server has been configured to send all tasks in a workflow to a single node, or to send tasks in a workflow block to a single node, as described in section 6.7, and the workflow or workflow block includes parallel non-exclusive tasks, then if these may run concurrently on the grid node.

By default, up to 10 such non-exclusive jobs can be run concurrently. This value can be changed in the "Maximum number of concurrent jobs" field, available in the "Server setup" area of the Job Distribution tab. That field is visible when the server mode "Single server" has been selected, as shown in figure 6.7. The value configured is passed through to the CLC Server queue with the grid worker.

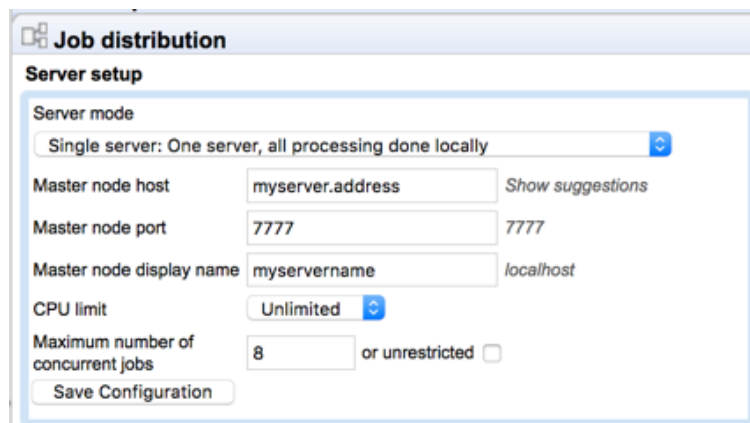


Figure 6.7: The Maximum number of concurrent jobs setting is visible when the Single server mode is selected.

A grid setup can be run with the Single server or Master node setting selected. To adjust the "Maximum number of concurrent jobs" if the Master node option is selected, temporarily change the mode to Single server, set the desired value, and then change the mode back to Master node.

Limitation: The maximum value that can be entered in the "Maximum number of concurrent jobs" field is the number of cores on the master server. Setting that maximum value is the equivalent of checking the unlimited box. If this value is smaller than the desired value, as might happen when grid nodes have many more cpu than the master server, then we recommend leaving this field blank so that the default value of 10 is used.

2. In any other context

Information about the CPU or thread requirements of the jobs must be passed to the grid scheduler. Non-exclusive algorithms expose their CPU or thread usage, and this information can be passed on to the grid scheduler via the `COMMAND_THREAD_MIN` and `COMMAND_THREAD_MAX` variables in the Shared native specification of a grid preset.

The variable `COMMAND_THREAD_MAX` would be used alone as an argument when a single value should be specified, or both the variables `COMMAND_THREAD_MIN` and `COMMAND_THREAD_MAX` can be provided when a range is required. An example of specifying a range is shown in the image of a grid present in section 6.3.7.

One can also use the functions `take_lower_of` and `take_higher_of` for settings relevant to configuring multiple job processing. For example, to specify 4 as the maximum number of cores to be used by a non-exclusive job, the following could be used as the argument to the relevant parameter in the Shared native specification of a grid preset: `{#take_lower_of COMMAND_THREAD_MAX, 4}`. As the non-exclusive job passes on its thread usage requirements via the `COMMAND_THREAD_MAX` variable, this evaluates to 4 if that requirement is higher than 4 or the value specified by the job if is lower than 4.

Further details about grid preset configuration, including Shared native specifications, functions and variables, can be found in section 6.3.7.

Licensing notes

Each CLC Grid Worker launched, whether it is to run alone on a node or run alongside a job already running on a particular node, will attempt to get a license from the CLC License Server. Once the job is complete, the license will be returned.

If the server has been configured to send all tasks in a workflow to a single node, only a single CLC Grid Worker will be launched for a given workflow run. Thus, irrespective of the number of concurrently running jobs in such a workflow run, only a single gridworker license is used.

If the server has been configured so that each task in a workflow is submitted separately, then a CLC Grid Worker will be launched for each task, resulting in the use of a gridworker license for each task, including non-exclusive jobs executed concurrently. When no licenses are available, jobs wait in the queue until a license becomes available.

If the server has been configured so that each block of a workflow is submitted to run on a single node, a CLC Grid Worker will be launched for each block. If the workflow contains no iteration blocks, then it, by definition, consists of a single block and will use a single gridworker license. If a workflow contains one or more iteration blocks, it will consume a number of licenses equal to the number of iterations of these blocks plus one for each additional, non-iterated block. See figure 6.13 in section 6.7 for more detail about workflow blocks.

6.3.10 Other grid worker options

Some java options can be set specifically for grid workers. This is done by creating a file called:

```
clcgridworker.vmoptions
```

and placing it in the same folder as the *deployed* `clcgridworker` script, that is, within the folder specified in the **Path to CLC Grid Worker** field of the grid preset. Each grid preset can have its own `clcgridworker.vmoptions` file.

Options that may be of particular use for grid workers include:

- `-Djava.io.tmpdir=<path>` Set the location where temporary files should be put.

- `-Dskip_lazytmp_cleanup=<boolean>` When set to true, `-Dskip_lazytmp_cleanup=true`, the grid worker will not attempt to clean up temporary data from previous analyses that, for whatever reason, were not cleared up previously. This option is intended for systems where temp areas for grid nodes are not local and the specified shared temp location is on a file system that does not support global file locking. As we highly recommend that temporary data areas are local, this option should rarely be of use.

For example, if a `clcgridworker.voptions` was created, containing the following line, it would, for the CLC Grid Worker specified in a given preset, set a temporary directory for the grid nodes, overriding the default that would otherwise apply:

```
-Djava.io.tmpdir=/path/to/tmp
```

Memory settings for grid workers If memory limits set using auto-detection, described in section 6.3.14, need to be overridden, then we recommend this be done using the **CLC Grid Worker memory limit** field of the grid preset configuration, as described in section 6.3.7. In earlier versions of *CLC Server*, a line of the form `-Xmx<value>` may have been added to a `clcgridworker.voptions` file to specify this limit. If setting limits in a grid preset, any `-Xmx` settings from `clcgridworker.voptions` files, should be removed, as values in these files will override those in a grid preset.

6.3.11 Testing a Grid Preset

There are two types of tests that can be run to check a Grid Preset. The first runs automatically whenever the *Save Configuration* button in the Grid Preset configuration window is pressed. This is a basic test that looks for the native library you have specified. The second type of test is optional, and is launched if the *Submit test job...* button is pressed. This submits a small test job to your grid and the information returned is checked for things that might indicate problems with the configuration. While the job is running, a window is visible highlighting the jobs progression as shown in figure 6.8.

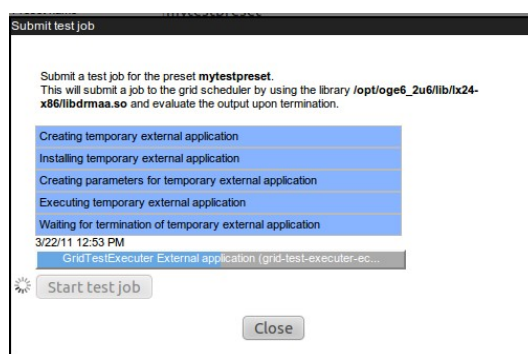


Figure 6.8: Testing a Grid Preset.

6.3.12 Client-side: starting CLC jobs on the grid

Starting grid jobs

Submitting jobs to grid nodes from a CLC Workbench

Once the *CLC Server* is configured and you are logged into it via a *CLC Workbench*, an extra option will appear in the first dialog box presented when setting up a task that could be executed on the *CLC Server*. At this stage, you can choose to execute the task on the machine the *Workbench* is running on, the *CLC Server* machine, or to submit the job to one of the available grid presets. To submit to the grid is as simple as choosing from among the grid presets in the drop down box, as shown in figure 6.9.

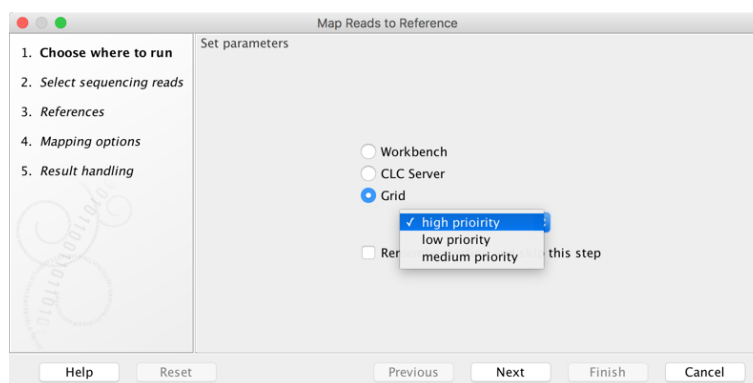


Figure 6.9: Starting the job on the grid.

Submitting jobs to grid nodes using the *CLC Server* Command Line Tools

Submitting jobs for execution on grid nodes using the **clcserver** command of the *CLC Server* Command Line Tools involves adding the **-G** parameter to the command, followed by the name of the grid preset to send the job to as the parameter value. A list of available grid presets is returned, along with other information about the **clcserver** command, if the command is run with just the server address, port and user credentials specified. Further details about the **clcserver** command can be found in the *CLC Server* Command Line Tools manual at https://resources.qiagenbioinformatics.com/manuals/clcservercommandlinetools/current/index.php?manual=Basic_usage.html.

6.3.13 Grid Integration Tips

If you are having problems with your *CLC Grid* Integration, please check the following points:

- Does your system meets the requirements of the *CLC Grid* Integration tool 6.3.2? For example, please check that the machine the *CLC Server* is running on is configured as a submit host for your grid system, and please check that you are running Sun/Oracle Java 1.7 on all execution hosts.
- The user running the *CLC Server* process is the same user seen as the submitter of all jobs to the grid. Does this user exist on your grid nodes? Does it have permission to submit to the necessary queues, and to write to the shared directories identified in the Grid Preset(s) and any `clcgridworker.vmoptions` files?
- Are your *CLC Server* file locations mounted with the same path on the grid nodes as on the master *CLC Server* and accessible to the user that runs the *CLC Server* process?
- If you store data in a database, are all the grid nodes able to access that database, using the user account of the user running the *CLC Server* process?

- If you store data in a database, did you enter a machine name in the Host box of the Database Location field when setting up the Database Location using the *CLC Server* web administration form? In particular, a generic term such as `localhost` will not work, as the grid nodes will not be able to find the host with the database on it using that information.
- If you installed the *CLC Server* as root, and then later decided to run it as a non-privileged user, please ensure that you stop the server, recursively change ownership on the *CLC Server* installation directory and any data locations assigned to the *CLC Server*. Please restart the server as the new user. You may need to re-index your *CLC* data locations (section 3.2.5) after you restart the server.
- Is your java binary on the PATH? If not, then either add it to PATH, or edit the `clcgridworker` script in the *CLC Server* installation area, with the relative path from this location: `gridres/dist/clcgridworker`, and set the JAVA variable to the full path of your java binary. Then re-save each of your grid presets, so that this altered `clcgridworker` script is deployed to the location specified in the **Path to CLC Grid Worker** field of your preset.
- Is the `SGE_ROOT` variable set early enough in your system that it is included in the environment of services? Alternatively, did you edit the *CLC Server* startup script to set this variable? If so, the script is overwritten on upgrade - you will need to re-add this variable setting, either to the startup script, or system wide in such a way that it is available in the environment of your services.
- Is your DRMAA library 64-bit? Both Java and DRMAA must be for 64-bit systems for it to work.

6.3.14 Understanding memory settings

Most work done by the *CLC Server* is done via its java process. However, some tools use external native binaries for the computational phases. These include those with a de novo assembly or mapping phases and those involving BLAST tools.

Java process

Each grid preset can have its own memory limit for the java process. This can be useful where separate queues are used for low overheads tasks, such as import jobs and trimming jobs, and high overhead tasks, such as de novo assemblies or read mappings.

Unless a memory limit is explicitly configured for a grid worker, auto-detection is used to determine the value to apply. This should be appropriate for most circumstances. The limit is determined as follows:

- If virtual memory is limited (`ulimit -v`), a quarter of that value or 50GB, whichever is smaller. Otherwise:
- If resident memory is limited (`ulimit -m`), half of that value or 50GB, whichever is smaller. Otherwise:
- Half of the amount of available physical memory or 50GB, whichever is smaller.

Order of priority for java process memory settings The first value found according to the list below will be applied:

1. A memory limit specified in a `clcgridworker.vmoptions` file. This method is not recommended.
2. A memory limit specified in a CLC Grid Preset. If values determined by auto-detection are not appropriate, this method can be used to specify a custom value. See section 6.3.7.
3. Auto-detection, as described above.

External binaries

Some tools make use of external binaries during one or more phases. Memory usage by external binaries is not restricted by limits set for the java process. For this reason, we recommend caution if you plan to submit jobs of these types to nodes that are being used simultaneously for other work.

6.4 Model III: Single Server setup

In this model, the master and execution node functionality is carried out by a single CLC Server instance. Here, the *CLC Server* software is installed on a single machine. Jobs submitted to the server are executed on this same machine.

To designate the system as a single server, after installation and starting the server, select the option `SINGLE_SERVER` from the drop down list of Server modes.

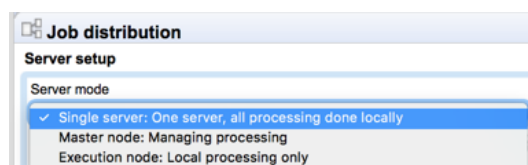


Figure 6.10: The configuration options for the types of machines running the **CLC Server**. The choices of relevance under normal circumstances are `SINGLE_SERVER` and `MASTER_NODE`. An administrator will not usually need to manually choose the Execution Node option. This option is there primarily to allow for troubleshooting.

You can then configure aspects of the server:

- **Master node host** - usually set to localhost for Single server mode. Click on the "Show suggestions" text next to this field to see information about the server that can be useful if localhost is not a suitable option for your setup.
- **Master node port** - usually 7777.
- **Master node display name** - the name shown in the top bar of the web interface for the server.
- **CPU limit** - The maximum number of CPU the CLC Server should use. This is set to unlimited by default, meaning that up to all cores of the system can be used.
- **Maximum number of concurrent jobs** - Limit the maximum number of jobs that are allowed to run concurrently on the single server. For further information about this setting see section 6.8.2.

The screenshot shows a web interface titled "Job distribution" with a sub-section "Server setup". The "Server mode" is set to "Single server: One server, all processing done locally". The "Master node host" is "myserver.address", "Master node port" is "7777", and "Master node display name" is "myservername". The "CPU limit" is "Unlimited" and the "Maximum number of concurrent jobs" is "8". There is a "Save Configuration" button at the bottom.

Figure 6.11: Configuring a single server.

6.5 Cloud settings

Cloud presets are configured in the Cloud settings area. Each cloud preset includes a job priority and information about how results should be handled. A tag can also be specified, which is then be added to all jobs submitted using that cloud preset. Users specify the cloud preset to use when submitting jobs to *CLC Genomics Cloud Engine* via their *CLC Workbench* or *CLC Server Command Line Tools*.

Before setting up cloud presets, please ensure the Cloud Server Plugin has been installed, and its plugin settings, which contain details of the cloud connection, have been configured.

The *Cloud Server Plugin* can be downloaded from <https://digitalinsights.qiagen.com/plugins/cloud-plugin/>.

Information about the *Cloud Server Plugin* settings is provided in the *Cloud Plugin* manual at: https://resources.qiagenbioinformatics.com/manuals/cloudplugin/current/index.php?manual=Configuring_AWS_CLC_Genomics_Cloud_Engine_settings.html.

6.6 Configuring cloud presets

A cloud preset controls characteristics of the job being submitted to a *CLC Genomics Cloud Engine* via a *CLC Server*, such as hardware requirements and whether the results should be automatically downloaded or not. Multiple presets can be configured. Users select the preset to use when they are launching a job

To create or edit existing cloud presets, log into the *CLC Genomics Server* web administrative interface and go to:

Job distribution | Execution node settings | Cloud settings

Click on **Add New Cloud Preset** and fill in a preset name, job tag (optional), hardware requirements and result handling strategy. The hardware requirements can be pre-filled based on available presets configured by the administrator of the *CLC Genomics Cloud Engine*.

Permissions for each cloud preset can be configured under the **Global permissions** tab.

6.7 Workflow queuing options

In the **Workflow queuing options** section under the Job distribution tab (figure 6.13), there are three options for how workflows should be submitted to nodes. These options reflect the three

organizational levels of workflows:

- **Tasks** The individual tasks that comprise the workflow
- **The whole workflow** All tasks in the workflow
- **Blocks** Sections of a workflow. For workflows without control flow elements, the entire workflow is a single block. For workflows with control flow elements:
 - Tasks downstream of an **Iteration** element and above a **Collect and Distribute** element form a block.
 - Tasks downstream of an **Iteration** element with no subsequent **Collect and Distribute** element form a block.
 - Linked workflow steps outside an iteration block form a block See figure 6.12.

Further details about control flow elements are provided in the Workflow chapter of the CLC Genomics Workbench manual available in html or pdf format from <https://digitalinsights.qiagen.com/technical-support/manuals/>

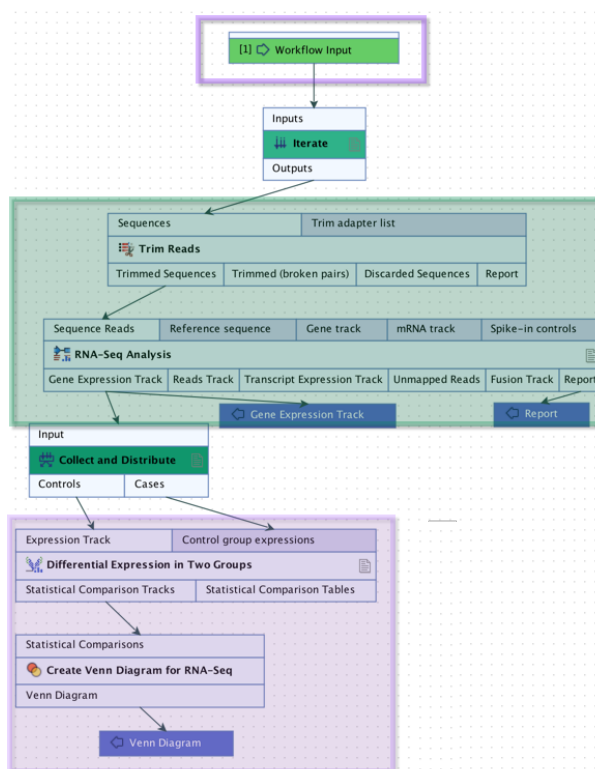


Figure 6.12: This workflow has one iteration block, shaded in turquoise, and one block after the iteration block, shaded in purple. It also has an optional block above the iteration block, outlined in purple. If a user chooses to import files as the initial action taken when launching this workflow, the import would be executed as an initial block. If they choose files already in a CLC File Location, the first block is the iteration block.

The workflow queuing options are:

- **Submit individual tasks to any available node** Each task of a workflow is scheduled separately for execution. For example, a workflow with 10 tasks would result in 10 jobs

being submitted. Each of those jobs can be sent to any available node with adequate resources when that step is ready to be run.

- **Submit all tasks to a single node** A single job submission is made for a workflow, regardless of how many tasks that workflow consists of. All tasks of that workflow are run on the same node. This option was previously called "Single entity".
- **Submit tasks in each workflow block to a single node** Each iteration of a block of a workflow, and each additional block outside iteration blocks, is scheduled separately for execution. Each job can be sent to any available node with adequate resources when that block is ready to be run. For workflows consisting of just one block, (no control flow elements), this option behaves just like the **Submit all tasks to a single node** option.

Further information about workflow queuing options is provided in section [6.7.1](#).

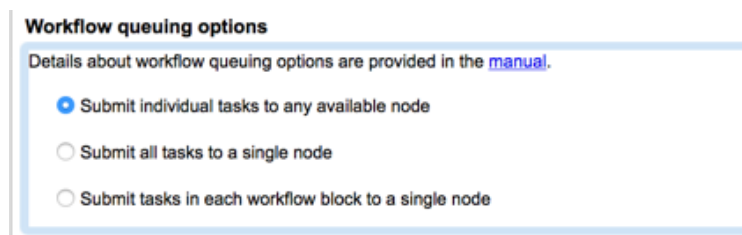


Figure 6.13: Workflow queuing options determine how workflow jobs are queued on servers with execution nodes.

6.7.1 Choosing a workflow queuing option

In general terms:

- With the **Submit individual tasks to any available node** option, each task is scheduled individually. Where large numbers of workflows are submitted and each workflow consists of several tasks, it can lead to a large scheduling overhead, with thousands of jobs being placed in the queue. However, on a multi-node system with spare capacity, this option provides the highest potential level of parallelization.
- With the **Submit all tasks to a single node** option, a single job submission is made for a workflow, regardless of how many tasks that workflow consists of, so scheduling overhead is minimized. However, only non-exclusive jobs within a workflow have the potential be executed in parallel.
- With the **Submit tasks in each workflow block to a single node** option, the scheduling overhead is low, with a single job submission per workflow block to be executed. Here, iterated workflow blocks have the potential to be executed in parallel on multi-node setups.

Further considerations relating to the choice of workflow queuing option include:

- Workflow blocks and full workflows run on a single node can leverage caching mechanisms, which aids performance.

On systems that frequently run at or close to capacity, the opportunity for gains through concurrent processing of parallel workflow tasks on multiple nodes is much lower than on a

system with spare capacity. So here, the performance gains using the **Submit all tasks to a single node** or **Submit tasks in each workflow block to a single node** option can outweigh those of submitting tasks separately, even when they are computationally intensive tasks.

- Where resource allocation is a focus, such as where many users are sharing the resources, the **Submit all tasks to a single node** option may help with resource access by different users.

For example, consider a grid node setup with 20 nodes, where one user submits 15 workflows with 10 tasks in each workflow. If each task is submitted as an individual job, those 150 jobs can be submitted across all 20 nodes. When the next user submits a job, it would be queued behind these 150 jobs. With the **Submit all tasks to a single node** option, the 15 workflows would have been sent to a maximum of 15 nodes, leaving 5 nodes available for the other user's job. Where workflows do not contain iteration blocks, the **Submit tasks in each workflow block to a single node** option would have the same effect.

- Blocks or entire workflows are only submitted to nodes capable of running all the included tasks. Where node hardware is not homogeneous or where certain job nodes have been dedicated to running only certain types of analyses, this should be considered when selecting the **Submit all tasks to a single node** or **Submit tasks in each workflow block to a single node** options.
- For grid node setups only: Where demand for gridworker licenses exceeds the number available, jobs wait in the queue until a license becomes available. The number of gridworker licenses needed to execute all tasks in a given workflow depends on the workflow queuing option selected.

With the **Submit individual tasks to any available node** option, the number of gridworker licenses needed equals the number of tasks. When the **Submit all tasks to a single node** option is selected, only one gridworker license will be needed for the whole workflow. This is also the case with the **Submit tasks in each workflow block to a single node** option when running workflows without an iteration block. For a workflow with one or more iteration blocks, the number of licenses used will be equal to the number of iterations of the blocks within the workflow plus one for each additional, non-iterated block.

6.8 Job running options

In the **Job running options** section, settings are available that affect how jobs are queued and run on single server and job node setups, as well as where intermediate results of workflows are stored.

6.8.1 Multi-job processing

There are three general categories of tools on the CLC Server: non-exclusive, streaming and exclusive, described in more detail below. Non-exclusive or streaming jobs can run concurrently alongside others of the non-exclusive type on a given machine. Those defined as exclusive cannot be run on the same server or node at the same time as other jobs of any type.

When the "Enable" option in the **Multi-job processing** area is selected, more than one analysis can run simultaneously on a CLC Server in single server mode or on a job node. This setting

Workflow queuing options

Details about workflow queuing options are provided in the [manual](#).

Submit individual tasks to any available node

Submit all tasks to a single node

Submit tasks in each workflow block to a single node

Job running options

Multi-job processing

Allow job nodes / single server to run multiple jobs at the same time. Restrictions apply, see [manual](#) for more information.

Enable

Disable

Fairness factor

For job nodes or single servers, set the maximum number of jobs that could overtake the one at the head of the queue before a job node is reserved for it. See [manual](#) for more information.

Concurrent jobs per node

Provide a value for the maximum number of jobs that can simultaneously run on each job node. See [manual](#) for more information.

No nodes attached

Intermediate workflow result handling

Select where to temporarily store intermediate workflow results. See [manual](#) for more information.

In the location final analysis results are stored

In a temporary directory

Figure 6.14: The default settings in the "Job running options" section of the administrative interface.

does **not** affect jobs sent to grid nodes. Concurrent job processing on grid nodes is described in section 6.3.9.

Running non-exclusive and streaming jobs concurrently on a single server or job node can be disabled by setting the "Multi-job Processing" option to "Disable" (figure 6.15). Click on **Save** to save changes to this setting.

Job running options

Multi-job processing

Allow job nodes / single server to run multiple jobs at the same time. Restrictions apply, see [manual](#) for more information.

Enable

Disable

Figure 6.15: The default status is to enable Multi-job processing. Select "Disable" to require that only a single job is executed at a given time on a job node or single server.

Non-exclusive, streaming and exclusive job types

- **Non-exclusive algorithms** Tools with low demands on system resources. They can be run alongside other jobs in this category, as well with alongside a job of the streaming category, described below. An example of a non-exclusive algorithm is "Convert from Tracks".

- **Streaming algorithms** Tools with high I/O demands, that is, much reading from and writing to disk is needed. These cannot be run with other jobs in the streaming category but can be run alongside jobs in the non-exclusive category. Examples of streaming algorithms are the NGS data import tools.
- **Exclusive algorithms** Tools optimized to utilize the machine they are running on. They have high I/O bandwidth, memory, or CPU requirements and therefore should not be run at the same time as other jobs on the same machine. An example is "Map Reads to Reference".

See Appendix section [17.4](#) for a list of *CLC Genomics Server* algorithms that can be run alongside others on a given machine.

6.8.2 Fairness factor

The fairness factor defines the number of times that a job in the queue can be overtaken by other jobs before resources are reserved for it to run. This setting affects the queue for single servers and job node setups.

In a situation where there are many non-exclusive jobs and some exclusive jobs being submitted, it is desirable to be able to clear the queue at some point to allow the exclusive job to have a system to itself so it can run. The fairness factor setting is used to determine how many jobs can move ahead of an exclusive job in the queue before the exclusive job will get priority and a system will be reserved for it. The same fairness factor applies to streaming jobs being overtaken in the queue by non-exclusive jobs.

The default value for this setting is 10. With this value set, a job could be overtaken by 10 others before resources are reserved for it that will allow it to run. A fairness factor of 0 means that a node will be reserved for the job at the head of the queue.

This value can be configured under the **Fairness factor** section of:

Admin  | **Job distribution**  | **Job queuing options**

6.8.3 Concurrent jobs per node

The maximum number of jobs that can be run on a single server or on each job node can be configured. The maximum allowable value is equal the number of cores on the relevant system. The default value is 10 or the number of cores on the system, whichever is lowest. If a CPU limit has been set on the single server or node, then the default is 10 or that CPU limit value, whichever is lowest.

Single server setup To configure the maximum number of jobs that can be run concurrently on a single server, go to the section **Server setup** under the Job Distribution tab of the web administration page. Enter the desired value in the box labeled "Maximum number of concurrent jobs" (figure [6.16](#)).

Job node setup To configure the maximum number of jobs that can be run concurrently on a given job node, go to the section **Job queuing options** under the Job Distribution tab of the web administration page. Enter a value for each job node listed under the "Concurrent jobs per node" section (figure [6.17](#)).

Server setup

Server mode
 Single server: One server, all processing done locally ▼

Master node host *master-host*

Master node port *7777*

Master node display name *master-host*

CPU limit ▼

Maximum number of concurrent jobs or unrestricted

Figure 6.16: Set the maximum number of concurrent jobs or check the "unrestricted" box. If unrestricted is chosen, the maximum number of jobs that can be run concurrently is equal to the number of cores on the system.

Concurrent jobs per node

Provide a value for the maximum number of jobs that can simultaneously run on each job node. See [manual](#) for more information.

host1-node01 or unrestricted

host2-node02 or unrestricted

Figure 6.17: Set the maximum number of concurrent jobs or check the "unrestricted" box for any job node. If unrestricted is chosen, the maximum number of jobs that can be run concurrently is equal to the number of cores on that job node.

6.8.4 Intermediate workflow result handling

Workflows contain a series of tasks, most of which produce data. Some data elements produced during a workflow execution are *intermediate results*. These are used temporarily, during the workflow run, to provide input to the next step of the analysis. Intermediate results are deleted once the workflow execution successfully completes.

Where intermediate results should be saved is controlled using the **Intermediate workflow result handling** options.

- **In the location final analysis results are stored** Intermediate results are stored in a subfolder of the output folder selected when the workflow is launched.
- **In a temporary directory** Intermediate results are stored in a temporary directory on the system the job is executed on, i.e. the single server, job node or grid node. This is usually faster than storing intermediate results under the output folder, particularly if the output folder is on a network drive. Note that if this option is selected, there must be enough temporary space to hold all the intermediate results on the systems that workflows are executed on.

Chapter 7

Status and management

Server operation can be managed from the Admin tab, under Status and Management (figure 7.1).

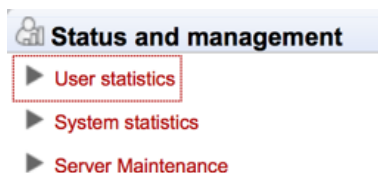


Figure 7.1: The Status and management tab.

7.1 User statistics

The User statistics section contains information about the number of users logged in, the number of active sessions (number of logins), and information about each active session. An example is shown in figure 7.2.

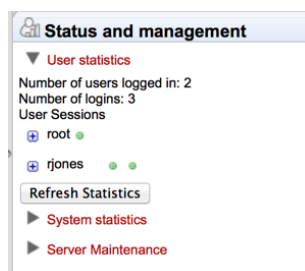


Figure 7.2: Information about the number of users and active sessions (logins) is provided in the User statistics area. Here, two users are logged in. rjones has two active sessions and root has one.

A green dot by a user's name indicates that they are logged into the server. Two green dots indicate that this user is logged in twice. For example, perhaps they have Workbenches running on two different systems and are logged in via both Workbenches. A grey dot means they have previously logged in but are not at this time.

Click on the small button with a plus to the left of a username to expand the information about that user's sessions (figure 7.3). You can also log users off the server by clicking on the **Invalidate Session...** button. This opens a confirmation dialog where a message to the user can

be written. This message is displayed via the user's active session. For example, if they are logged into a Workbench, a window will pop up saying they have been logged out of the server and also containing the message written in this field. This action forcibly logs the user out of the *CLC Server*. This action does **not** stop jobs already submitted or running on the server. Optionally, you can send a message to the user whose session is being terminated (see figure 7.4). If the user is logged into the *CLC Server* from a *CLC Workbench*, then the message entered will appear in a warning box that pops up via the *CLC Workbench*.



Figure 7.3: Details about *jbloggs*' session can be seen by clicking on the small button to the left of that username.

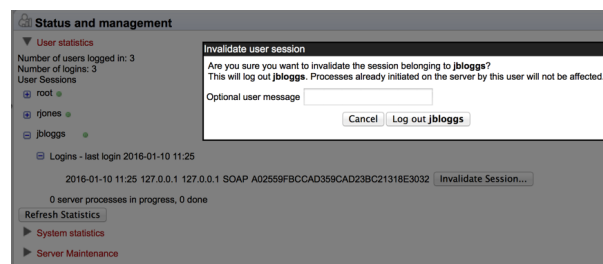


Figure 7.4: Clicking on the *Invalidate Session* button will forcibly log a user out of the *CLC Server*. The admin can optionally provide a message to the user when doing this.

7.2 System statistics

Crashed threads, suggesting system level problems, are reported in this area. In some instances, a system restart may be needed to resolve the issue.

The message "No system level problems detected" is shown in this area if no problems have been detected. An example of the information provided when a problem is detected is shown in figure 7.5. In the case shown, the job submission threads were dead, with the problem reported here and in more detail in the *CLC Server* log files.

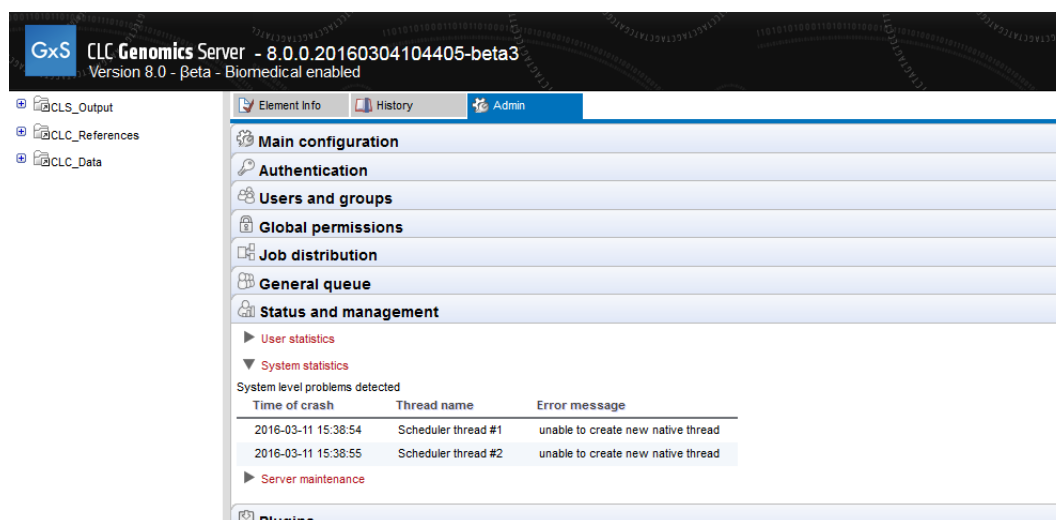


Figure 7.5: System level problems detected and reported in the system statistics area.

7.3 Server maintenance

Settings under the Server maintenance tab allow a server administrator to change the operating mode of the server and send out messages to users of the *CLC Server* (see figure 7.6).

- **Normal Operation** The *CLC Server* is running.
- **Maintenance Mode** Current jobs are allowed to run and complete, but submission of new jobs is restricted. While the server is in maintenance mode, users already logged in can check the progress of their jobs or view their data, but they cannot submit new jobs. Users not already logged in cannot log in. An administrator can write a warning message, for example, to inform users about the expected period of time the server will be in maintenance mode.
- **Log Out Users** All users currently logged in will be logged out. All running jobs will be allowed to complete. No users can log in while in this mode. An administrator can also write a warning message for the users.
- **Shut down** The *CLC Server* and any attached job nodes will shut down.
- **Restart** The *CLC Server* and any attached job nodes will be shut down and restarted.

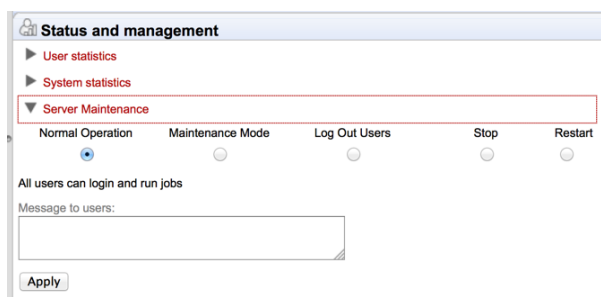


Figure 7.6: The server administrator can control the operating mode of the *CLC Server* from under the *Server maintenance* tab.

Chapter 8

Queue

Clicking the **Queue** panel will show a list of all the processes that are currently in the queue including jobs in progress.

An example is shown in figure 8.1.

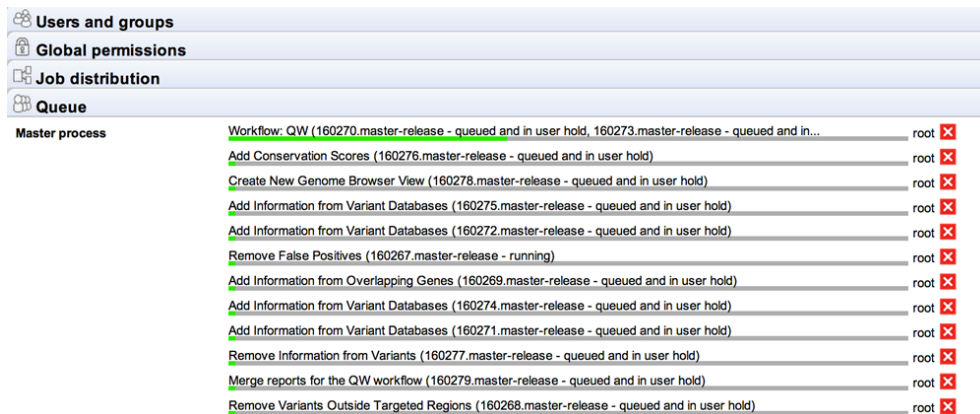


Figure 8.1: The process queue.

For each process, you are able to **Cancel** (☐) the processes. At the top, you can see the progress of the process that is currently running.

Chapter 9

Audit log

The audit log records the actions performed on the *CLC Server*. Included are actions like logging in, logging out, import, and the launching and running of analysis tasks. Data management operations such as copying, deleting and adding files are not Server actions and are thus not recorded.

Audit log information is available via the web administrative interface under the **Audit log** tab. The information presented here is stored in a database. Once a month, and when the *CLC Server* is started up, entries in the audit log older than 3 months are deleted.

The limit the audit log database can grow to is 64 GB. If a new entry will push the size past this limit, the system will remove some of the oldest entries so that it is possible for newer entries to be added.

Audit information is also written to text-based log files. Upon the first activity on a given date, a new log file called `audit.log` is created. This file is then used for logging that activity and subsequent Server activities on that day. When this new `audit.log` file is created, the file that previously had that name is renamed to `audit.<actual events date>.log`. These log files are retained for 31 days. When the creation of a new `audit.log` file is triggered, audit log files older than 31 days are checked for and deleted.

The audit log files can be found under the Server installation area under `webapps/CLCServer/WEB-INF`.

The audit log text files are tab delimited and have the following fields:

- Date and time
- Log level
- Operation: Login, Logout, Command queued, Command done, Command executing, Change server configuration, Server lifecycle; more may be added and existing may be changed or removed.
- Users
- IP Address
- Process name (when operation is one of the Command values) or description of server lifecycle (when operation is Server lifecycle)

- Process identifier - can be used to differentiate several processes of the same type.
- Status - can be used to identify whether the entry was successful or not, e.g. if a job execution failed it will be marked here. Any number other than 0 means failed.

Chapter 10

Server plugins

Download and install server plugins and server extensions

Plugins, including server extensions (commercial plugins), are installed by going to the **Extensions** (🔧) tab in the web administrative interface of the single server, or the master node of a job node or grid node setup, and opening the **Download Plugins** (📁) area (figure 10.1).

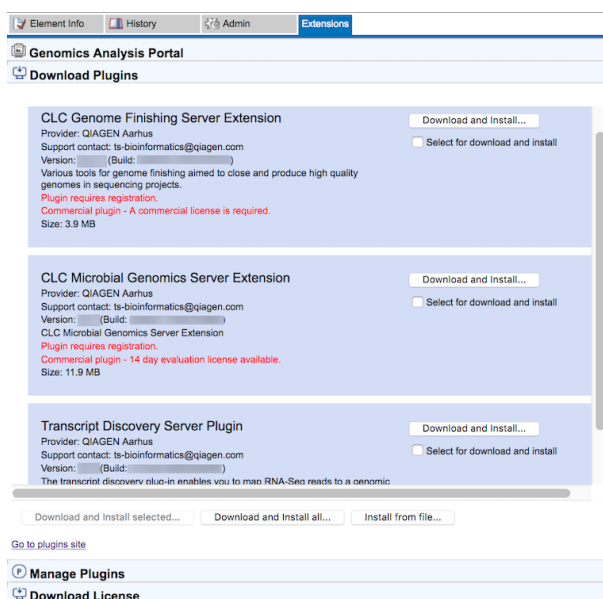


Figure 10.1: Installing plugins and server extensions is done in the Download Plugins area under the Extensions tab.

If the machine has access to the external network, plugins can be both downloaded and installed via the CLC Server administrative interface. To do this, locate the plugin in the list under the **Download Plugins** (📁) area and click on the **Download and Install...** button.


To download and install multiple plugins at once on a networked machine, check the "Select for download and install" box beside each relevant plugin, and then click on the **Download and Install All...** button.

If you are working on a machine without access to the external network, server plugin (.cpa) files can be downloaded from: <https://digitalinsights.qiagen.com/products->

[overview/plugins/](#) and installed by browsing for the downloaded file and clicking on the **Install from File...** button.

The *CLC Server* must be restarted to complete the installation or removal of plugins and server extensions. All jobs still in the queue at the time the server is shut down will be dropped and would need to be resubmitted. To minimize the impact on users, the server can be put into Maintenance Mode. In brief: running in Maintenance Mode allows current jobs to run, but no new jobs to be submitted, and users cannot log in. The *CLC Server* can then be restarted when desired. Each time you install or remove a plugin, you will be offered the opportunity to enter Maintenance Mode. You will also be offered the option to restart the *CLC Server*. If you choose not to restart when prompted, you can restart later using the option under the **Status and Management** tab.

For job node setups only:

- Once the *master CLC Server* is up and running normally, then restart each *job node CLC Server* so that the plugin is ready to run on each node. This is handled for you if you restart the server using the functionality under the **Server Maintenance** area under the **Admin**  tab.
- In the web administrative interface on the *master CLC Server*, check that the plugin is enabled for each job node.



Installation and updating of plugins on connected job nodes requires that direct data transfer from client systems has been enabled. See section 3.4 for details.

Grid workers will be re-deployed when a plugin is installed on the master server. Thus, no further action is needed to enable the newly installed plugin to be used on grid nodes.

Links to related documentation

- Maintenance Mode: section 7
- Restarting the server: section 2.7.1
- Plugins on job node setups: section 6.2.3
- Grid worker re-deployment: section 6.3

Managing installed server plugins and server extensions

Installed plugins are managed and can be uninstalled from under the **Manage Plugins**  area figure 10.2 of the **Extensions**  tab.

As when installing plugins, the *CLC Server* must be restarted to complete the action. See above for links to further information.

The list of tools delivered with a server plugin can be seen by clicking on the **Plugin contents** link to expand that section. Workflows delivered with a server plugin are not shown in this listing.

Plugin compatibility with the server software

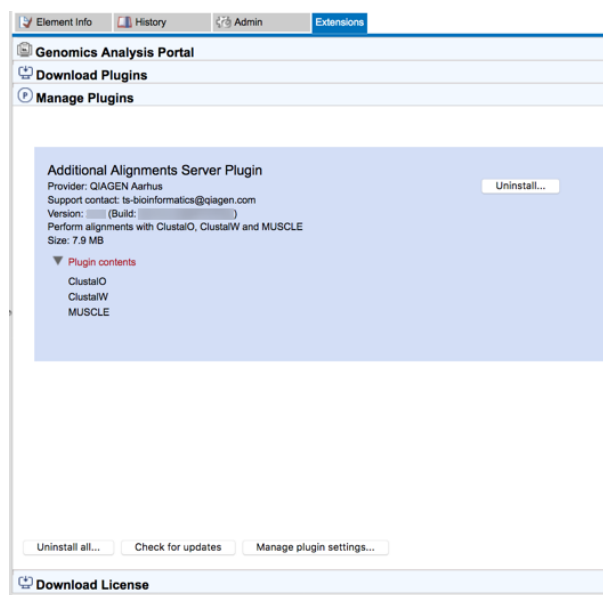


Figure 10.2: Managing installed plugins and server extensions is done in the *Manage Plugins* area under the *Extensions* tab. Clicking on *Plugin contents* opens a list of the tools delivered by the plugin.

The version of plugins and server extensions installed must be compatible with the version of the *CLC Server* being run. A message is written under an installed plugin's name if it is not compatible with the version of the *CLC Server* software running.

When upgrading to a new major version of the *CLC Server*, all plugins will need to be updated. This means removing the old version and installing a new version.

Incompatibilities can also arise when updating to a new bug fix or minor feature release of the *CLC Server*. We recommend opening the **Manage Plugins** area after any server software upgrade to check for messages about the installed plugins.

Server extension licensing

Commercial plugins, known as server extensions, require a license to be installed in the *CLC Server* before analysis tools delivered by the extension can be used. The license only needs to be present on the master server on grid and job node setups¹. If a license file is present, but it is valid only for an older version of the plugin, or it has expired, a warning will be shown.

Please refer to the appendix of the individual commercial plugin manuals for detailed information about licensing of that product.

¹Prior to *CLC Genomics Server* 11.0, module licenses were also required on nodes.

Chapter 11

BLAST

The *CLC Server* supports running BLAST jobs submitted from the workbenches that have BLAST tools and from *CLC Server Command Line Tools*. Users will be able to select data from Server **data locations** (see section 3.2.1) to search against other sequences held in Server data locations, or against BLAST databases stored in an area configured as an **import/export directory** (see section 3.3).

11.1 Adding directories for BLAST databases on the Server

In the web interface of the server, you can configure your Server for BLAST databases:

Admin (🔑) | **BLAST Databases** (🔑)

Here, you can add a folder where you want the Server to look for BLAST databases. However, before doing this, please ensure that the folder you will be adding has been configured as an **import/export directory** (see section 3.3). This is necessary because BLAST databases are not truly CLC data, and thus are stored outside data locations specified for CLC data. They need, however, to be stored somewhere accessible to *CLC Server* process though, hence the need to put them in a directory configured as an import/export directory.

After the folder holding BLAST databases is configured as an Import/Export directory, it can be configured as a location that the *CLC Server* will look in for BLAST databases.

Do this by clicking on the **Edit BLAST Database Locations** button at the bottom of the area under the BLAST Databases area in the administrative interface.

This will bring up a dialog as shown in figure 11.1 where you can select which of the import/export directories you wish to use for storing BLAST databases.

Once added as a BLAST Database Location, the *CLC Server* will search this directory for any BLAST databases and list them under the BLAST tab in the web interface (see a section of this as an example in figure 11.2).

This overview is similar to the one you find in the Workbench BLAST manager for local databases including the following information:

- **Name.** The name of the BLAST database.

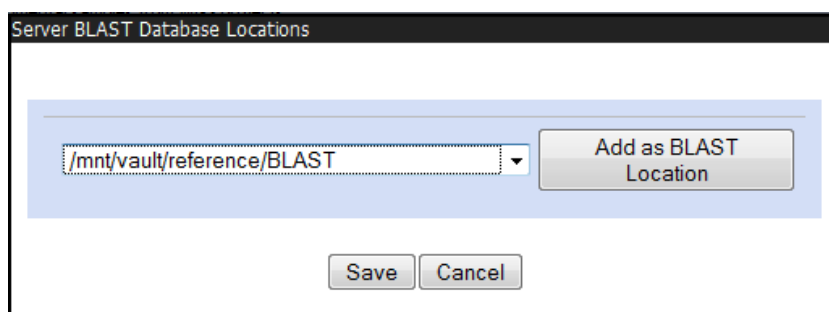


Figure 11.1: Adding import/export directories as BLAST database locations.

BLAST Databases				
BLAST databases overview				
Name	Description	Date	Sequences	Type
NC_000001	Human makeDB test	2011-11-14	19	DNA
all_contig	Homo sapiens build 37.3 genome database (reference assembly GRCh37.p5 [GCF_000001405.17] and alternate assemblies HuRef [GCF_000002125.1] and CRA_TCAGchr7v2 [GCF_000002135.2])	2011-10-07	4900	DNA
allcontig_and_rna	mouse build 37 RNA, reference and alternate assemblies	2011-05-25	35640	DNA
alt_CRA_TCAGchr7v2_contig	alt_CRA_TCAGchr7v2_contig	2011-10-07	6	DNA
alt_HuRef_contig	alt_HuRef_contig	2011-10-07	4530	DNA
alt_contig	Mus musculus build 37 genome database (alternate assembly Mm_Celera only)	2010-11-09	13033	DNA

Figure 11.2: Selecting database to BLAST against.


- **Description.** Detailed description of the contents of the database.
- **Date.** The date the database was created.
- **Sequences.** The number of sequences in the database.
- **Type.** The type can be either nucleotide (DNA) or protein.
- **Total size (1000 residues).** The number of residues in the database, either bases or amino acid.
- **Location.** The location of the database.

To the right of the Location information is a link labeled Delete that can be used to delete a BLAST database.

11.2 Adding and removing BLAST databases

Databases can be added in two ways:

- Place pre-formatted databases in the directory selected as BLAST database location on the server file system. The CLC Server will automatically detect the database files and list the database as target when running BLAST. You can download pre-formatted database from e.g. <ftp://ftp.ncbi.nih.gov/blast/db/>.

- Run the **Create BLAST Database** () tool via your Workbench, and choose to run the function on the Server when offered the option in the Workbench Wizard. You will get a list of the BLAST database locations that are configured on your Server. The final window of the wizard offers you a location to save the output to. The output referred to is the log file for the BLAST database creation. The BLAST databases themselves are stored in the designated BLAST database folder you chose earlier in the setup process.

A note on permissions: To create BLAST databases on the Server, using the Workbench interface, the user **running the CLC Server process** must have file system level write permission on the import/export directory that you have configured to hold BLAST database.

By default, if you do not change any permissions within *CLC Server*, all users logging into the *CLC Server* (e.g., via their Workbench, or via the Command Line Tools), will be able to create BLAST databases in the areas you have configured to hold BLAST databases.

If you wish to restrict the ability to create BLAST databases to these areas completely, but still wish your users to be able to access the BLAST databases to search against, then set the file system level permissions on the import/export directory so they are read-only.

When listing the databases as shown in figure 11.2, it is possible to delete the databases by clicking the **Delete** link at the far right-hand side of the database information.

Chapter 12

External applications

Non-interactive command line applications and scripts can be integrated into the CLC environment by configuring them as *external applications*. Once configured and installed, external applications are available to launch via the graphical menu system of a CLC Workbench or via the CLC Server Command Line Tools. External applications can also be included in workflows, allowing complex, reproducible analyses involving CLC tools and other, non-CLC tools to be easily configured and launched by end users.

There are two types of external application:

- **Standard external applications**, where a command line application is run directly on the server system.
- **Containerized external applications**, where an application is executed from within a Docker container. Containerized external applications are only supported on Linux-based *CLC Server* setups.

The *CLC Server* administrator controls which tools are made available as external applications, which parameters are adjustable when launching the tool, and who should have access.

Figure 12.1 shows an overview of the actions and data flow that occur when a standard external application is launched on the *CLC Server* via a *CLC Workbench*. The data flow can be summarized as follows:

1. An end user specifies input data and sets values for parameters when launching the external application from a *CLC Workbench* or *CLC Server Command Line Tools*.
2. The *CLC Server* exports the input data from the *CLC Server* to a temporary file.
3. The *CLC Server* launches the underlying application (standard external applications) or the container containing the underlying application (containerized external applications), and provides the parameter values specified by the user and the input data from the temporary file. The underlying tool or container runs as a separate process to the *CLC Server*. That process is owned by the same user that owns the *CLC Server* process.
4. When the command line application has finished, results are handled as specified in the external application configuration. Usually this involves results being imported into the CLC

environment and saved to the location specified by the user when the external application was launched.

- Results imported into the CLC environment are available for viewing and further analysis, for example using a *CLC Workbench*.

Temporary files are created outside the CLC environment during the execution of third party (non-CLC) tools and are deleted after the process completes.

Integration with External Application (Server Side)

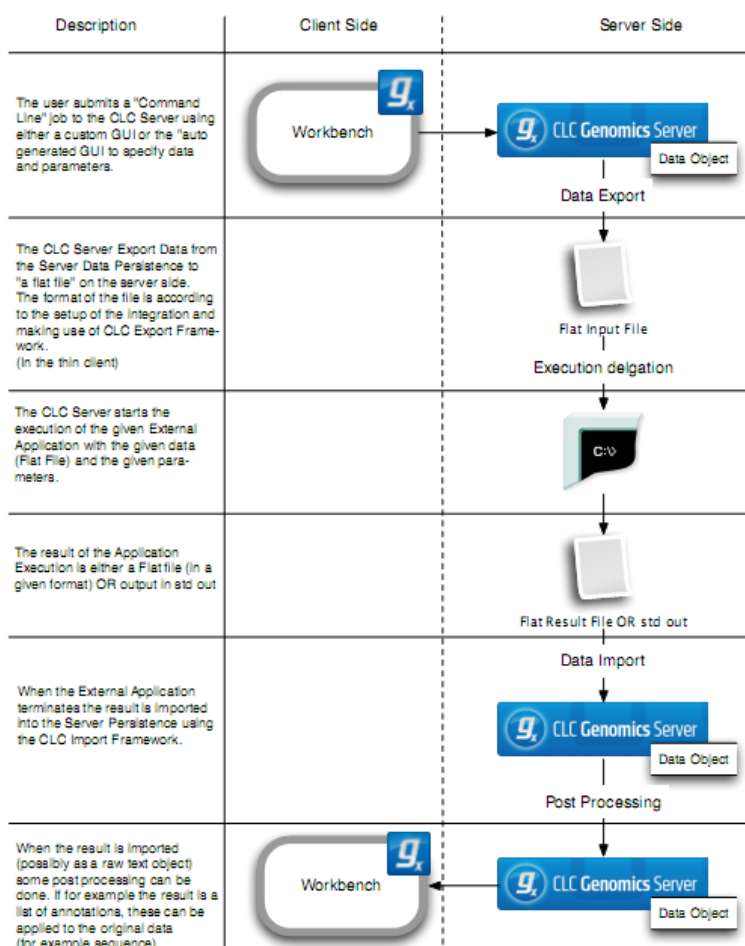


Figure 12.1: An overview of the flow of a standard external application when launched from a CLC Genomics Workbench.

Key information about external applications

- The CLC Server software should be run by an unprivileged user. Like other CLC Server tasks, external applications processes are owned by the same logical user that owns the CLC Server process itself. If the system's root user is running the CLC Server process, then tasks run via the External Applications functionality will also be executed by the root system user. This is usually undesirable.
- For a standard external application, the underlying tool must be available on all the systems where an external application can be run by the CLC Server.

- For containerized external applications, it is sufficient that the containerized execution environment is configured on all the systems where the external application can be run.
- An external application configuration must be saved before it is available for use via a *CLC Workbench* or *CLC Server Command Line Tools*. Configurations stored in the Drafts area are not made available for use.
- A folder called "External Applications" appears in the *CLC Workbench* Toolbox menu when a *CLC Workbench* is connected to a *CLC Server* with available external applications.
- Updates to existing external application configurations are registered in the *CLC Workbench* during a single login session. To discover new external applications from a client application, you must log out of and back into the *CLC Server*.

12.1 External application configurations

Individual external applications and the containerized execution environment are configured under the **External applications** tab of the web administrative interface (figure 12.2).

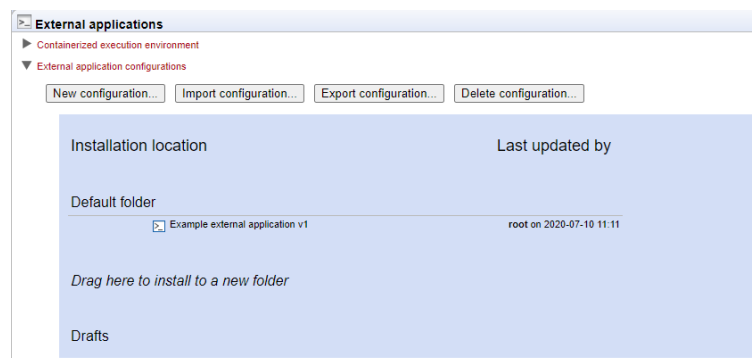


Figure 12.2: Individual external applications and the containerized execution environment are configured under the *External applications* tab.

For quick reference:

- Configuration of the containerized execution environment is described in section 12.1.1.
- Creating and editing external application configurations is described in section 12.2.
- Importing and exporting external application configurations is described in section 12.4.
- Including external applications in workflows is described in section 12.9.
- Launching external applications is described in section 12.10.
- Suggestions for troubleshooting external applications are provided in section 12.11.

12.1.1 Configuring the containerized execution environment

To run containers as external applications, the containerized execution environment must be enabled and configured. This is done under the *External applications* tab (figure 12.3). The full docker command executed when a containerized external application is launched combines the

"docker" command with parameters configured here, followed by the parameters specified in individual external command configurations, as described in section 12.2.

Containerized external applications are only supported on *CLC Server* systems running on Linux. Currently, we support Docker containers.

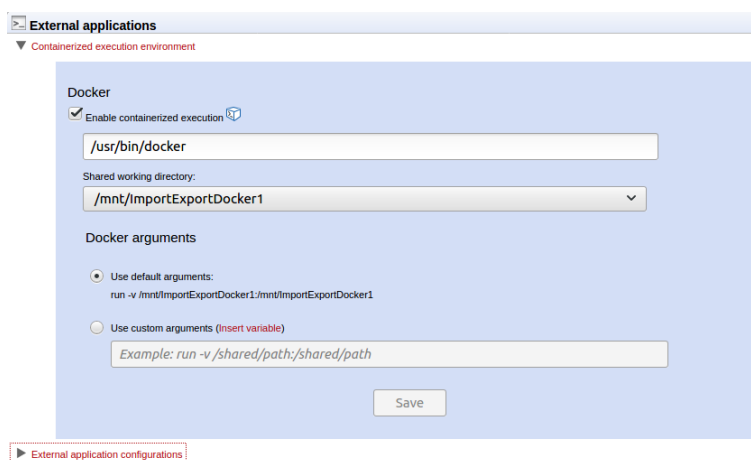


Figure 12.3: The server's container execution environment is configured under the External applications tab.

To enable the execution of containerized external applications, check the **Enable containerized execution** checkbox.

To configure the *CLC Server* for executing containers as external applications, expand the **Containerized execution environment** area (figure 12.3), and:

- Enter the full path to the Docker client in the top field.
Note that the user running the *CLC Server* application must have permission to run the docker executable.
- Select the **Shared working directory** from the drop-down list of import/export directories.
This directory will be bind mounted into the container launched and used to exchange data between the container and the *CLC Server*. This directory must therefore be shareable between the containers and the system that the *CLC Server* is running on.
Configuring import/export directories for the *CLC Server* is described in section 3.3.

- Specify the arguments to be passed to the docker command when a containerized external application is launched on this server setup. Arguments specific to particular external applications are specified in the individual external application configurations.

- **Use default arguments** With this option selected, the "-v" parameter is passed to docker followed by the shared working directory on the host system, selected above, and a mount point within the container, separated by a colon. The initial part of any command executed for containerized external applications will take the form:

```
docker run -v <import-export-dir>:<mount-point-in-image>
```

For convenience, the mount point in the container is set to be the same as the shared working directory location on the host system. If you wish to specify a different mount point, select the "Use custom arguments" option, described below, instead.

- **Use custom arguments** All arguments specified here are passed to docker when a containerized external application is launched. This list of arguments *must* include the "-v" option followed by the path to the shared working directory selected above and a mount point within the container, separated by a colon. Any environment variables specified here are considered *system variables* set for the running *CLC Server*.

Note: Environment variables can also be specified *for individual external applications*, as described in section 12.2.5. These are system variables set on the external application process started by the *CLC Server*.

12.2 Configuring external applications

External applications are created and configured in the *CLC Server* web administrative interface. Creating and editing external applications is described in section 12.2.1. Existing configurations can also be exported and imported. This is described in section 12.4.

Note: Immediately after creating and saving an external application configuration, that external application will be made available for use by client software by default. To keep the external application hidden, drag it to the Drafts area.

12.2.1 Editing external applications

Creating and editing external applications is done in a dedicated editor (figure 12.4). To open this editor, log into the *CLC Server* web administrative interface, open the **External Applications** tab, expand the "External applications configuration" area, and then either double click on the name of an existing external application or click on the **New configuration...** button.

Figure 12.4: Different aspects of an external application are configured under each tab of the external application editor. The "External command" tab is where the command to run and its parameters are entered and configured.

An overview of the type of information configured under each of the editor tabs is provided below, along with links to more detailed information:

External command: The name of an external application, as seen by end users, the type of the

external application (standard or containerized), the command line including its parameters, further configuration of parameters with names within curly brackets (section 12.2.2).

High-throughput sequencing import / Post-processing Where relevant to the external application, configuration of NGS importer or other CLC post-processing tools that should act on the results of the command line application (section 12.2.3).

Stream handling The handling of information sent to the standard out and standard error streams by the underlying application (section 12.2.4).

Environment Environment variables that should be present for the external application when it executes (section 12.2.5).

End user interface Settings affecting how an external application is displayed in a *CLC Workbench* client (section 12.2.6).

Management Settings relating to the status of the external application (draft or installed) and other management tasks (section 12.2.7).


12.2.2 External command

The sections under the **External command** editor tab (figure 12.4) are:

External application name The name seen in the *CLC Workbench* Toolbox menu and given to the corresponding workflow element for this external application. This name is also used as the basis of the name to use to launch the external application using the *CLC Server Command Line Tools*.

Command line The command run when the external application is launched. The information to provide differs for standard external applications and containerized external applications, and is described in more detail below for each case.

Parameters values that should be substituted at run time are written within *{curly brackets}*. This includes parameters that should be configurable by the end user. Other parameters and values are written as normal in this field.

General configuration Parameter values specified in *{curly brackets}* in the **Command line** field will have a corresponding entry in the **General configuration** area. There, these values are configured, including specifying their type, and for some types, configuring the values to use or to be offered to end users to select from. The description of a parameter can be configured by clicking the tooltip icon () next to the parameter. The description will be displayed in clients, for example as a tooltip when running the external application from the *CLC Workbench*, or in the help listed for this application via the *CLC Server Command Line Tools*.

External application type External applications can be "Standard (non-containerized)", or "Containerized: Docker". Standard external applications are executed directly on a server system. Containerized external applications are run from within containers.

To run containerized external applications, the containerized execution environment must be enabled and configured, as described in section 12.1.1.

Command lines for *standard* external applications

The **Command line** field should contain the path to the application and all parameters to be passed to that application. For illustration, a simple example of the cp (copy) command with 2 positional parameters is shown in figure 12.4.

Command lines for *containerized* external applications

The **Command line** field should contain *only* the parameters to send to docker that are *not already configured for the containerized execution environment*, described in section 12.1.1. These will usually be aspects of the command specific to running the individual external application.

For example, for a container with a command that takes one argument, the information written in this field could take the form:

```
<image-identifier> <command-to-run-from-image> <parameter>
```

The full docker command executed when an external application is launched combines the information configured for the containerized execution environment with the information provided in the Command line field. So, for example, if the default configuration settings for the containerized execution environment were used, the full docker command run when this external application is launched would take the form:

```
docker run -v <import-export-dir>:<mount-point-in-image> \
  <image-identifier> <command-to-run-from-image> <parameter>
```

In figure 12.5, the command for a containerized external application running the alignment program MAFFT is shown as an example. That example is described in more detail in section 12.8.

Figure 12.5: The command line for a containerized external application contains an reference to the image, here the repository and tag have been used, but it could also be the image identifier, followed by the command to run from the container and the parameters to provide to that command. Here there is a single parameter, written in curly brackets, indicating that the value will be substituted at run time.

Parameter value types

Details of parameter value types are outlined below. A brief description is also provided in the web administrative interface when a value type is selected and the mouse cursor is hovered over it. Particularly important types for external application configurations are **User-selected input data (CLC data location)**, which is the usual choice for parameters specifying input data, and **Output file from CL**, which is the usual choice for specifying results generated by the underlying application.

- **Text** - The end user can provide text that will be substituted into the command at runtime. A default value can be configured.
- **Integer** - The end user can provide a whole number that will be substituted into the command at runtime. A default value can be configured. If no value is set, then 0 is the default used.
- **Double** - The end user can provide a number that will be substituted into the command at runtime. A default value can be configured. If no value is set, then 0 is the default used.
- **Boolean text** - A checkbox is shown in the Workbench wizard interface. If the user checks the box, the given text will be substituted into the command at runtime. If the box is unchecked, this means that no value will be substituted.
- **CSV enum** - A drop down list is presented to a Workbench end user, from which they can choose a desired option. The corresponding value will be substituted into the command at runtime. To configure this parameter type, enter a comma delimited list of the values to be substituted at runtime into the first box, and a comma delimited list of corresponding labels to display to end users in the second box. Each entry in a given list should be unique and the two lists should be of equal length.

For an example of this, please see section 12.6 on setting up Velvet as an external application.

- **User-selected input data (CLC data location)** - The end user should specify one or more input files from those stored on the *CLC Server*. In the General configuration area, the appropriate exporter should be selected, so that the format of the data is will be as needed for the command line application. Each exporter can be configured further by clicking on the **Edit parameters** button, shown in figure 12.4¹. A window then appears with a list of configurable parameters, as shown in 12.6.

Choices to make when configuring export parameters include:

- Default values to be applied when the external application is run. To edit fields that are locked by default, click on the symbol of the lock image to open the lock. Once unlocked, changes can be made.
- Which parameters end users will be able to configure when launching the external application. A parameter with an unlocked symbol beside it will be displayed to the end user and its value will be editable. Locked parameters are not shown and cannot be changed by end users.

¹Configurable export parameters were introduced with CLC Genomics Server 10.0.

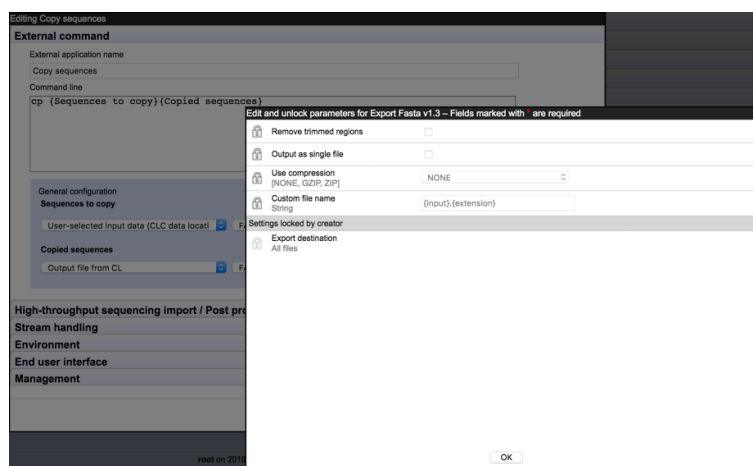


Figure 12.6: Clicking on the *Edit parameters* button for the "Sequences to copy" parameter brings up a window with the editable parameters for the selected exporter. Parameters with a locked symbol beside them are not shown to, and are thus not configurable by, the end user.

- **User-selected files (Import/Export directory)** - The end user should specify one or more input files stored in an Import/Export area configured on the CLC Server. This option is used to specify files not in a CLC location. Files can be configured so they are pre-selected for the end user, but the end user can deselect pre-configured files when launching the external application.
- **Output file from CL** - This option should be used for parameters that define an output of the external command line application. Once selected, a drop down list appears with options for how the output should be handled:
 - **Where results should not be imported into the CLC Server**, choose the option *No standard import or map to high throughput sequencing importer*.
 - **To import results into the CLC Server using a high throughput sequencing (NGS) importer**, choose the option *No standard import or map to high throughput sequencing importer* and then configure the importer to use under the **High-throughput sequencing import / Post processing tab**, described in section 12.2.3.
 - **To import the results using a standard importer**, choose the importer to use from the drop down list presented. If the import type **Automatic** is selected, the importer used is determined by the filename suffix in combination with a check of the format of the elements in the file. If the file type is not recognized, it will be imported as an external file. A list of file formats, including the expected filename suffix for each format, can be found in the appendix of the CLC Genomics Workbench manual: Read more about search here: http://resources.qiagenbioinformatics.com/manuals/clcgenomicsworkbench/current/index.php?manual=Local_search.html.

The third, empty field can be used to enter the name of the file the external process is expected to produce. If left blank, the base name of the file produced by the command line tool will be used as the base name for the data element imported into the CLC Server. Specifying a default filename in the third field, including the relevant suffix (e.g. .fasta, .xlsx), is recommended.

When **Output file from CL** is selected for at least one value, the end user will need to provide a location on the *CLC Server* to store results. This will be the case even if the output of the external file will not be imported, as log files will still be written to the location selected.

- **File** - The end user should specify input files from their local machine. These are typically not CLC files. The *CLC Server* must be configured to allow direct data transfer from client systems for this option to be usable. If it is not, the parameter will not be configurable by the end user and they will see a message saying server upload is disabled when they try to launch the external application.
- **Context substitute** - The options are:
 - *CPU limit max cores* The core limit defined for the server that executes the command will be substituted.
 - *Name of user* The name of the user who launched the external application will be substituted.

This parameter is not visible to the end user.

- **Boolean compound (legacy)** - This is a legacy option, which is no longer recommended for use and will be removed in a future release.

A very simple configuration illustrating parameter configuration is shown in figure 12.4 for the *cp* command. In the **General configuration** area, the *Sequences to copy* parameter is set to **User-selected input data (CLC data location)** meaning that the end user will specify the data to be copied from a CLC File Location. That data will be exported to a fasta format file. The *Copied sequences* parameter is set to type **Output file from CL**, indicating that this is the output from the command, and the standard fasta importer was selected for importing the results into the *CLC Server*.

A tip for exploring how many files an exporter will generate

A simple way to explore how many files an exporter will generate with a given configuration is to set up an external application using the *echo* command and a single parameter linked to the exporter of interest. Configure the "Standard out handling" option, selecting the "Plain text" option, described in section 12.2.4. The output from such an external application is a file, which is re-imported into the *CLC Server* as a text file. This file contains the full paths to the files the exporter created.

If an exporter is configured in a way that will lead to multiple output files, then the full path to each output file will be substituted in the command at runtime. The external application itself must be able to handle the outputs generated.

12.2.3 High-throughput sequencing import / Post-processing

Data generated by the external tool can be imported using a high throughput sequencing importer or processed after import by a post processing tool on the *CLC Server*. To configure a high throughput sequencing importer or post processing tool:

- Choose the option **Output file from CL** for a parameter value in the **General configuration** area under the **External command** tab.
- Choose the option "No standard import or map to high throughput sequencing importer". Despite the name, this will also allow connections to be made to post processing tools.
- Open the **High-throughput sequencing import / Post processing** tab.
- Click on the **Add new** button.
- Select the high throughput sequencing import or post processing tool of interest from the list.
- Click on the button below the list called **Edit and map parameters...**. This button appears when a tool is selected.

A new window showing all the parameters for that tool will appear. See figure 12.7 for an example.

- Select the relevant external application parameter to be used as input to the tool by clicking on it in the list.

For high throughput sequencing tools, the input parameter is usually called "Selected files". For post processing tools, the name of the input field varies, but the word "(input)" is usually present by that parameter name.

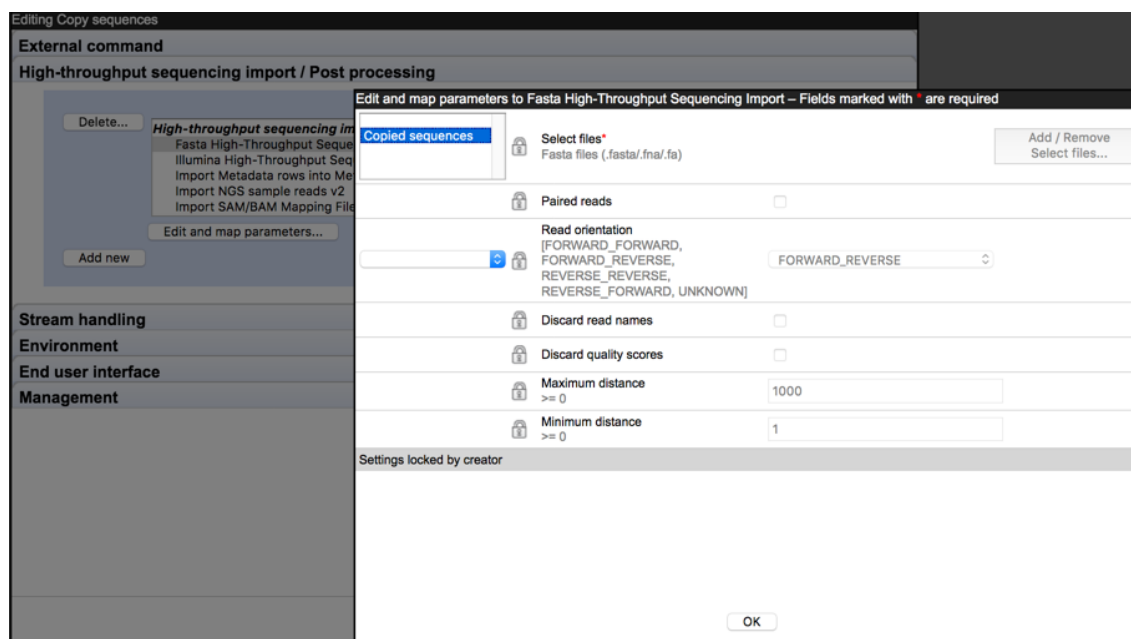


Figure 12.7: Clicking on the "Edit and map parameters..." button opens a window for configuring the selected tool. Here, the parameter "Copied sequences" has been selected by clicking on it, thereby specifying that the file associated with that parameter should be used as input to the tool. All the parameters here have a locked symbol beside them, so none of them will be editable or shown to end users.

- Configure any of the other parameters that you wish to, for example:
 - Change the parameter values. To edit fields that are locked by default, click on the symbol of the lock image to open the lock, then make changes.

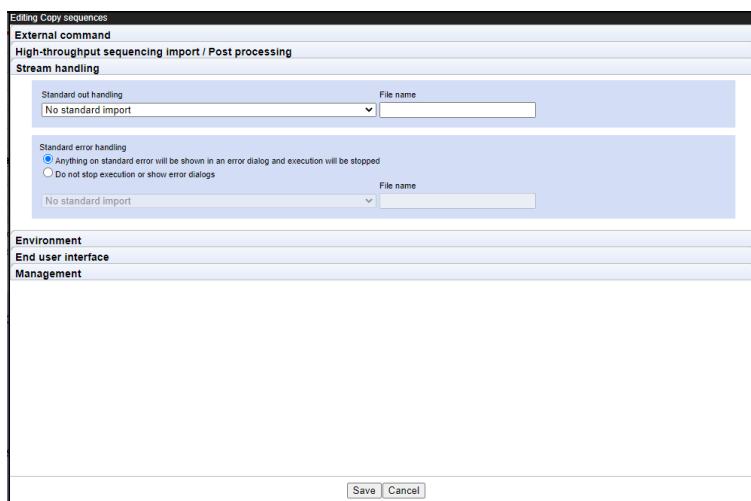
- Unlock parameters that should be visible and editable by end users by clicking on the lock symbol.

After configuration changes are saved, text in the General Configuration panel will be updated, making it clear which tool has been selected for use with a given command parameter. For example, if the post processing tool: "Import SAM/BAM Mapping Files" was configured and the relevant output mapped to it, the text in the General configuration area for that output would show: "Linked with Import SAM/BAM Mapping Files" in the second field.

If you change your mind about linking to a high throughput sequencing importer or post processing tool from an external application parameter, you must remove the connection between the two. This would usually be done by deleting the relevant configuration in the High-throughput sequencing import / Post processing area.

12.2.4 Stream handling

Handling standard out and standard error streams for the external application is configured under the **Stream handling** tab, shown in figure 12.8.



The screenshot shows a configuration window titled "Editing Copy sequences". It has several tabs: "External command", "High-throughput sequencing import / Post processing", and "Stream handling". The "Stream handling" tab is active and contains two sections. The first section, "Standard out handling", has a dropdown menu set to "No standard import" and a "File name" text input field. The second section, "Standard error handling", has two radio buttons: "Anything on standard error will be shown in an error dialog and execution will be stopped" (which is selected) and "Do not stop execution or show error dialogs". Below these radio buttons is another "File name" text input field. At the bottom of the window are "Save" and "Cancel" buttons.

Figure 12.8: How standard out and standard error should be handled is configured under the **Stream handling** tab.

The contents of standard out can be ignored or imported into the *CLC Server* using a standard importer. For applications where standard out contains the main result, choosing an appropriate importer would generally make sense. It can also be useful to import information sent to standard out for debugging purposes. In the **File name** field, the name of the raw file used to temporarily store the output from standard out must be specified.

By default, if information is sent to standard error by an application, the tool is stopped and the information is reported to the end user. The contents of standard error can instead be imported into the *CLC Server* by selecting the option **Do not stop execution or show error dialogs**. If the contents of standard error are imported, the **File name** must be specified in the same way as for standard out.

The names entered into the **File name** fields for standard out and standard error handling are visible to end-users, without a file extension, in the following places:

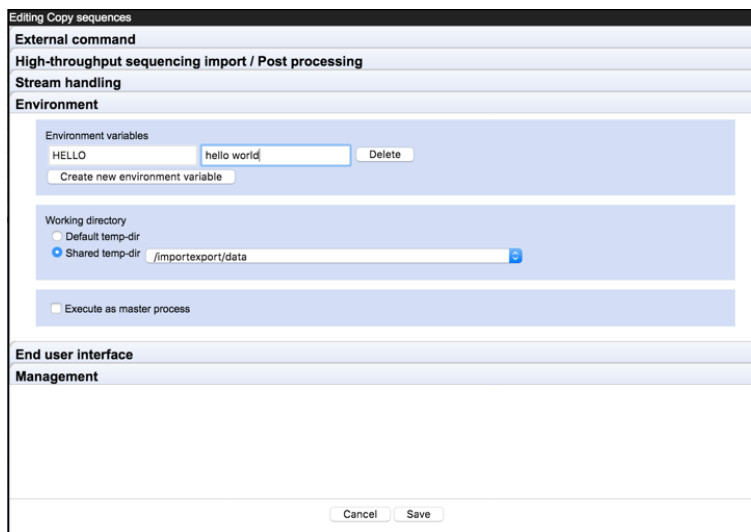
- This name is given to the data element imported into the *CLC Server*.
- This name is used as the label for the output channel of the workflow element corresponding to the external application.
- This name is the default name for output elements connected to the relevant workflow output channels.

12.2.5 Environment

Aspects of the environment within which the external application will be run are configured under the **Environment** tab.

Environmental variables

Environment variables that should be present for the external application when it executes can be created here, and default values set. In the example shown in figure 12.9, an environment variable named "HELLO" with value "hello world" would be present in the execution environment of the external application.



The screenshot shows a dialog box titled "Editing Copy sequences" with several tabs. The "Environment" tab is active. It contains the following sections:

- External command:** High-throughput sequencing import / Post processing
- Stream handling:** (empty)
- Environment:**
 - Environment variables:** A table with one row: HELLO | hello world | Delete. Below it is a "Create new environment variable" button.
 - Working directory:** Two radio buttons: "Default temp-dir" (unselected) and "Shared temp-dir" (selected). Next to "Shared temp-dir" is a text field containing "/importexport/data".
 - Execute as master process:** An unchecked checkbox.
- End user interface:** Management

At the bottom of the dialog are "Cancel" and "Save" buttons.

Figure 12.9: Under the *Environment* tab, settings related to the environment an external application will be run on are configured.

Working directory

The **Working directory** setting specifies where temporary files should be created. This setting is only relevant to standard (non-containerized) external applications. For containerized external applications, the working directory is defined in the containerized execution environment, as described in section section 12.1.1.

Default temp-dir Temporary files will be placed under the directory specified by the `java.io.tmpdir` setting for the system.

Shared temp-dir Temporary files will be placed under the directory you specify. The files will be accessible to all execution nodes and the master server without needing to be moved between machines.

To be available for use as a shared temp-dir, a directory must be:

- Already configured as an *Import/export directory*, as described in section 3.3.
- A shared directory, accessible by all machines where the external application will be executed.

Grid environments: For an external application to be executable on grid nodes, the *Shared temp-dir* option must be chosen for the working directory.

Job node setups: For an external applications to run on job nodes, either Working directory option is fine. However, if the directory specified by `java.io.tmpdir` is not an area shared between machines, and it usually is not, choosing *Default temp-dir* means that files will need to be moved between the master and job nodes.

Execute as master process

When the **Execute as master process** option is enabled, the command line application will be executed on the master machine of a job node or grid setup. Export, import and post-processing steps are still run on the execution environment selected by the user when launching the external application. This setting has no effect for single server setups, where all execution happens on the same system.

With this option unselected, all stages of the external application are run on the execution environment selected when launching the external application. This is the default situation.

Execute as master process is not recommended for use with memory or cpu intensive tasks as the command line application will be launched on the master system without consideration of how busy that system is, or what processing capabilities it has.

For grid setups: Whether or not the **Execute as master process** option is enabled, export, import and post-processing steps will be run on a grid node if a grid execution environment is selected when launching an external application. This is why the Working directory option must be set to *Shared temp-dir* when running an external application on a grid setup.

12.2.6 End user interface

Settings under the *End user interface* tab (figure 12.10) affect the external application presentation in a *CLC Workbench* client:

- **Parameters per wizard step:** The number of parameters to present in a given wizard step when the application is launched. The default value is 4. With this value, up to 4 parameters will appear on each wizard page that the user steps through when launching the job.
- **Toolbox subfolder name:** The name of a subfolder under the *CLC Workbench* Toolbox | External Applications folder, where the external application should be listed. If a subfolder of the specified name does not already exist, it will be created. When this field is empty, the application will be listed directly under Toolbox | External Applications.

Subfolder organization is also reflected under the main External applications tab, where the configurations are grouped according to subfolder. External applications without a subfolder specified are placed in the *Default folder* area. Configurations in draft status are always placed in the *Drafts* area, no matter what the subfolder designation is.

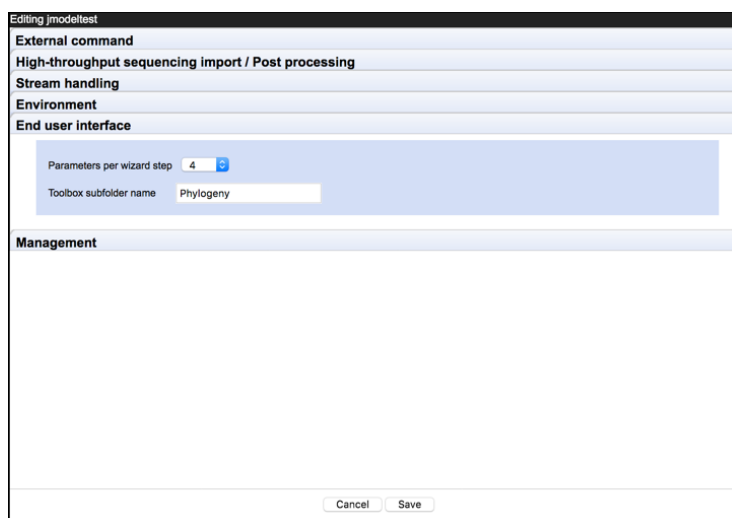


Figure 12.10: End user interface settings affect how the external application is presented in a CLC Workbench client.

Additional notes:

- The text entered is case sensitive; "foldername" and "Foldername" refer to 2 different subfolders.
- The creation of subfolders of subfolders is not supported. If you enter text like "myfolder/subfolder", a single folder of exactly that name would be listed under the External Applications folder in the Workbench Toolbox.
- Dragging external application configurations between *Installation locations* under the External applications tab has the effect of updating the subfolder configuration. The new location in the Toolbox will be seen by end users when they next log into the CLC Server from the CLC Workbench.

Other configuration aspects that affect CLC Workbench end user experience

The following aspects of an external application configuration are seen when using a CLC Workbench client:

- Under the External command tab, the external application name is the name displayed under the Toolbox menu and is used as the name of the corresponding workflow element.
- Under the External command tab, the name entered for parameter values between *{curly brackets}* is used as:
 - A parameter label in the launch wizard
 - A parameter name for the CLC Server Command Line Tools
 - The name of the output channel of the external application workflow element.

- Under the Stream handling tab, the file names entered for standard out and standard error handling are used as the names of output channels for the external application workflow element.
- Where a default value is specified, that value is generally displayed in the launch wizard.
- The parameters listed in exporter configuration windows are *all* those available for the exporter. By default, these are all locked, and thus are not shown to end users when the external application is launched. Unlocking some of these can sometimes make sense, but unlocking all of them can result in a confusing, and sometimes conflicting, set of options for end users.

12.2.7 Management

Information about an external application is provided under the **Management** tab, and following general management tasks can be configured here:

- Choose to install the external application on the *CLC Server* or keep it as a draft. Installed applications are available for use by client software. Those stored as drafts are not.
- Delete the external application configuration entirely. This does not affect the underlying tool the external application was configured for.
- Create a copy. Copies of installed or draft external applications can be made. The copy will be given a version number of 1 and placed in the same folder as the original.

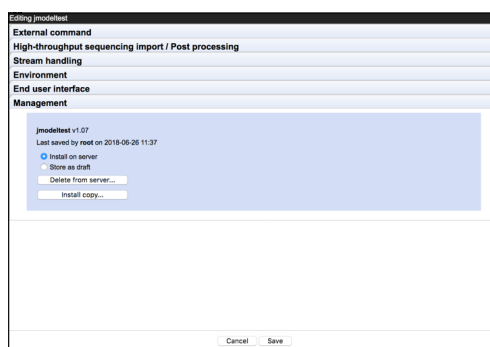


Figure 12.11: Under the Management tab, information about an external application is provided and general management configuration options are available.

12.3 Using consistent reference data in external applications

For external applications that include third party tools that use reference data, such as reference genomes, annotations, primer sets, etc., the same reference data should be used for both the third party and CLC processing steps. To achieve this, reference data must be in locations and formats that can be used by each relevant application. This usually means either importing reference data into a *CLC Server* or exporting it from a *CLC Server* and placing it where the third party application can access it when it is run.

Reference data is imported into a *CLC Server* using client software, either a *CLC Workbench* or the *CLC Server Command Line Tools*. Data to be imported should be copied into an Import/export directory first, from where it can be imported.

If you do not already have the reference data you need, the Reference Data Manager of the CLC Genomics Workbench can be used to download data from QIAGEN servers and some public repositories such as Ensembl to the *CLC Server*. Further details about this can be found in section 3.2.2.

Reference data is exported from a *CLC Server* using standard export functionality of the client software, where the relevant data elements are selected in the Navigation Area of a *CLC Workbench*, or specified using CLC URLs when using the *CLC Server Command Line Tools*. Exported data is put into an import/export directory, from where it can be moved to the location of your choice.

Import/export directories are configured under the Main tab of the server web administrative interface, as described in section 3.3.

Data import and export are described in the client software manuals: <https://digitalinsights.qiagen.com/technical-support/manuals/>.

12.4 Import and export of external application configurations

External application configurations can be exported from or imported into a *CLC Server*, facilitating backup and exchange.

Exporting external application configurations

To export external applications configurations, click on the **Export configuration. . .** button.

To export the external application configurations as an XML file to be saved on disk, choose "Export to local file", then select the relevant applications and click on the **Export** button (figure 12.12). This will produce a single XML file containing the configurations of the selected external applications. This XML file can then be imported, for example if you are sharing the configurations with others, or wish to reinstate an earlier version of the configurations.

For standard external applications, this configuration file is all that is needed. For containerized external applications, the containerized execution environment settings are *not* included in this XML file.

It is also possible to export the XML configuration file directly to a cloud location in Amazon S3. To do this, the *Cloud Server Plugin* must be installed on the *CLC Server*, and the parameter "S3 URL for exporting external applications" must be configured in the plugin settings. Once the XML file has been exported to a cloud location in Amazon S3, *CLC Workbench* setups with the *Cloud Plugin* installed can import it from that location. Once that is done, workflows containing external applications can be submitted from the *CLC Workbench* to run on a *CLC Genomics Cloud Engine* without needing to also connect to a *CLC Server*.

Importing external application configurations

External application configuration files can be imported to a *CLC Server* by clicking on the **Import configuration. . .** button. In the window that appears, click on the **Browse** button and select the configuration file to import. Then click on the **Import and add External Applications configuration** button.

A dialog is then presented confirming the import. If the imported file included the configuration of

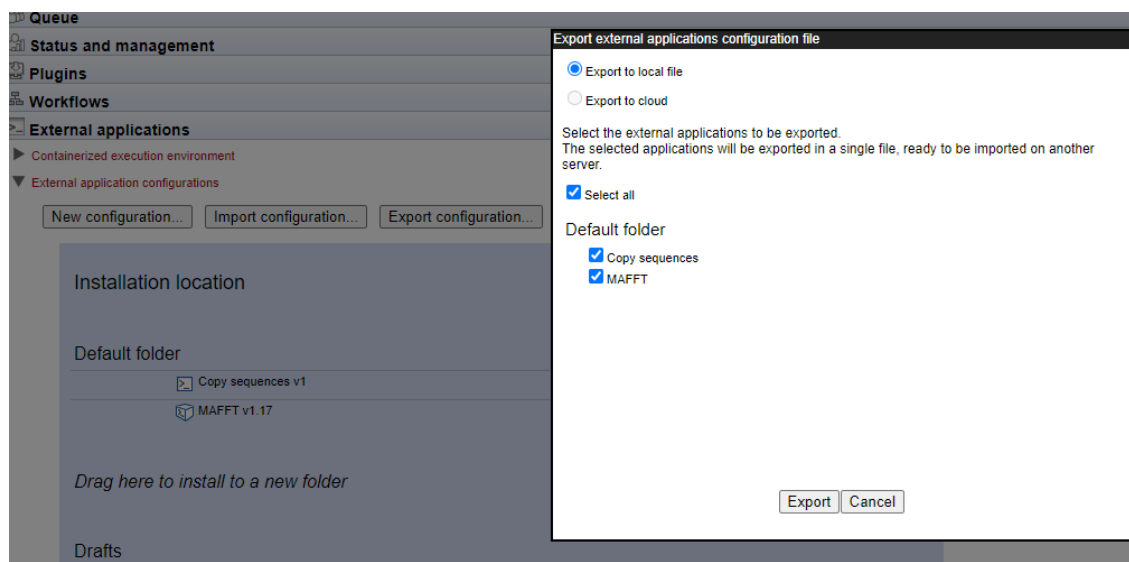


Figure 12.12: The configurations for two external applications will be exported after the Export button is clicked upon.

an external application with the same internal ID as one already on the *CLC Server* and they are different versions, the copy already on the server will be overwritten. The confirmation dialog will include the names of any external applications overwritten.

12.5 Updating external application configurations

When an external application is run, data is exported from the *CLC Server* and results are imported into the *CLC Server*. If the versions of the exporters and importers differ between the external application configuration and the *CLC Server*, the external application configuration will need to be updated. This can happen when upgrading to a new server version or when importing external applications configuration files generated on an older server.

When updates to exporters or importers are needed for published external applications, a button labeled **Updates are needed** appears in the "External application configurations" area (figure 12.13). Red exclamation marks are also displayed next to the individual external applications that need to be updated, and within the external application editor, beside the name of the tab where the update is needed, usually the "High throughput importers/Post processing" tab, and also under the Management tab.

Configurations can be individually updated. Alternatively, click on the **Updates are needed** button. This brings up the "Update External Applications" window, which contains a list of the configurations that need updating. Clicking on the **Update** button in that window will update all the configurations that can be auto-updated. Mouse over the name of individual external applications to see information about what needs to be updated.

Any configuration that cannot be updated from the "Update External Applications" window has to be updated manually. An example where a configuration cannot be auto-updated is where a tool has been replaced. These are relatively rare events.

Note: The need for updates is not reported for external application in the Drafts area and these external applications are not listed in the "Update External Applications" window.

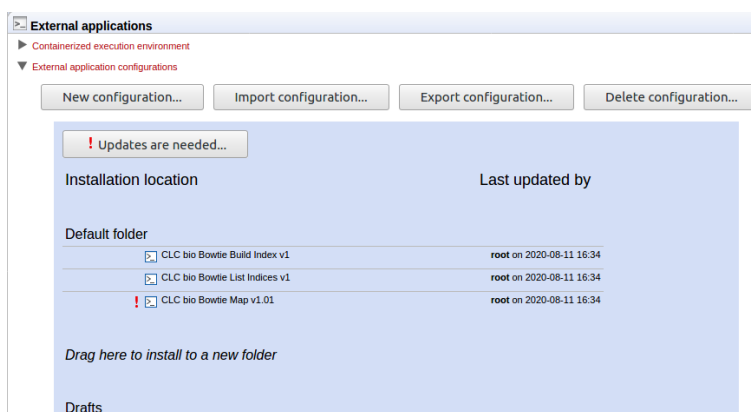


Figure 12.13: The CLC bio Bowtie Map external application needs updating, as indicated by the exclamation mark by its name. The "Updates are needed" button is visible, reflecting this. Clicking on that button allows us to auto-update all (possible) external application configurations in a single action.

Under the Management tab, the most recent auto-update carried out on an external application configuration is recorded separately to the latest update made manually. If there has been at least one auto-update carried out, clicking on the button labeled **View last auto-update changes** will show information about what was done (figure 12.14).

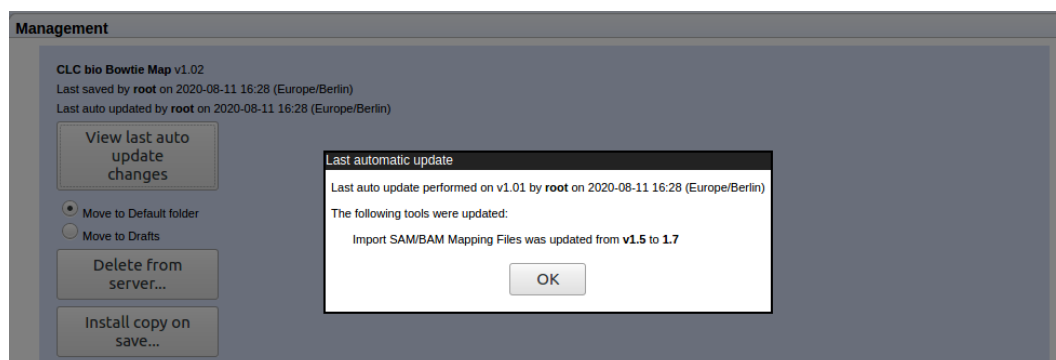


Figure 12.14: If auto-updates have been carried out, details of the latest one can be viewed under the Management tab of the external application configuration editor. Here, the View last auto-update changes button has been clicked, revealing information about what was done.

12.6 Example: Velvet (standard external application)


In this example, we configure Velvet [Zerbino and Birney, 2008], a popular de novo assembler for next-generation sequencing data, as a standard external application.

The Velvet package includes two programs that need to be run consecutively. The external applications system on the CLC Server is designed to call one program, so a wrapper script is needed to make the needed consecutive calls to the Velvet applications.

An example script as well as a configuration file are available in a zip file at <https://resources.qiagenbioinformatics.com/external-applications/velvet-example.zip>. These will be used to illustrate how this sort of application can be configured as an external application on a CLC Server.

12.6.1 Installing Velvet

To get started, you need to do the following:

- Install Velvet on the server computer. The program and installation information is available from <https://github.com/dzerbino/velvet/tree/master>. If you have job nodes, Velvet will need to be installed on all the nodes that will be configured to run it.
- Download the scripts and configuration files from <https://resources.qiagenbioinformatics.com/external-applications/velvet-example.zip>. These files have been created assuming that Velvet is installed in `/usr/local/velvet`. If it is installed elsewhere, please update the files with the correct path to the program on your server.
- Check to ensure execute permissions are set on the `velvetg` and `velveth` executable files in the Velvet installation directory. These must be executable by the user that owns the CLC Server process.
- Unzip the `velvet-example.zip` file and place the `clcbio` folder and its contents in the Velvet installation directory. This contains a script (`velvet.sh`) that links the two Velvet programs, `velvetg` and `velveth`, together. If the Velvet binaries are not in the folder `/usr/local/velvet`, you will need to edit the line that starts with `exe=` to include the correct path.
- Set the permissions on the `velvet.sh` script in the `clcbio` subfolder so that it can be executed by the user that owns the CLC Server process.
- Import the `velvet.xml` configuration file: Log into the server via the web administrative interface and go to the **External applications**  tab. Expand the "External applications configuration" section and click on the **Import Configuration. . .** button.
After the configuration file has been imported, an external application named **CLC bio Velvet** will appear in the "Default folder" area for the external applications configurations. Click on the **CLC bio Velvet** name. An external application editor should open, with the External command tab open, as shown in figure [12.15](#).
- Update the path to the Velvet installation at the very top if necessary.

If you wish to execute this job on grid nodes, then a shared temp-dir must be specified in the Working directory section of the Execution area of the configuration. See section [12.2.5](#) for details.

If you see a small red exclamation point beside the external application name, then something is wrong and needs to be attended to. The specific area where there is a problem should also be identified by a red exclamation mark. This is seen, for example, when the versions of a High-throughput sequencing import or Post-processing step specified in the configuration file is different to the version on the *CLC Server*. This can occur when the configuration was set up on an older version of the *CLC Server* than the one running. Rectifying this is straight forward, and is described in section [12.5](#).

12.6.2 Running Velvet from the Workbench

To run Velvet, open a Workbench and connect to a server where the Velvet external application is installed. Then:

Figure 12.15: The Velvet configuration after the external application configuration file has been imported.

- Go to:
 - Toolbox | External Applications (📁) | CLC bio Velvet (🔍)**
- Confirm where you wish to run the job.
- Select (📁) the reads to assemble and configure the Velvet parameters, as shown in figure 12.16.

Figure 12.16: Configuring Velvet parameters from a Workbench.

- Click **Next**.

- Specify where to save the results.
- Click **Finish**.

The process that follows has four steps:

1. The sequencing reads are exported by the server to a fasta format file. This is a temporary file that will be deleted when the process is done.
2. The velvet script is executed using the fasta file and the user-specified parameters as input.
3. The resulting output file is imported into the save location specified in the save step of the Workbench dialog, and the user is notified that the process is done.
4. All temporary files are deleted

12.6.3 Understanding the Velvet configuration

The Velvet configuration file is explained here as a specific example of all external application configuration files.

Going back to figure 12.15, there is a text field at the top. This is where the command expression is created, in this case:

```
/opt/local/velvet/clcbio/velvet.sh {hash size} {read type}
      {reads} {expected coverage} {contigs}
```

The first part is the path to the script. The following parts are parameters that are interpreted by the server when calling the script. Parameters to be interpreted are surrounded by curly brackets { }. Note that each parameter entered in curly brackets gets an entry in the panel below the command line expression.

The first parameter, `hash size`, can be entered as a **Double** (which is a number that can take decimal values in computer parlance). The user provides a value when they launch Velvet. A default value is provided in the configuration (31).

The second parameter is `read type`, which has been configured as a **CSV enum** which means a list of possible values that the user can choose from. The first part of the configuration information consists of the parameters to be used when calling the velvet script (`-short`, `-shortPaired`, `-long`, `-longPaired`), and the second part is the more human-readable representation that is to be shown in the Workbench (`Short`, `Short Paired`, `Long`, `Long Paired`).

The third parameter is `reads` which is used for the input data. When the **User-selected input data** option is chosen, a list of all the available export formats is presented. In this case, Velvet expects a fasta file. When a user starts Velvet from the Workbench, the server starts exporting the selected input data from `clc` format to a temporary fasta file before running the script.

The `expected coverage` parameter is similar to `hash size`.

The last parameter, `contigs`, represents the output file, as indicated by the choice of "Output file from CL" as the type. Here, you specify how the output from velvet should be handled. A

list of standard import formats is provided, as well as the option not to import using those tools. Choosing not to import using those tools means that you can choose a high throughput importer instead from the section High-throughput sequencing import/ Post-processing section.

For this example, Do not import is the action set for the contigs parameter. Then, below, in the High-throughput sequencing import/ Post-processing section, the Fasta High-throughput Sequencing Import tool has been selected. Thus, when the results from velvet are ready, they are imported into the CLC Server using that tool and saved where the user indicates when they run the job.


12.7 Example: Bowtie (standard external application)

In this example, we show how to integrate Bowtie [Langmead et al., 2009], a popular tool for mapping short sequencing reads to a reference sequence, as a standard external application. Here, two post processing tools will be configured, allowing us to import more than one output generated by bowtie into the CLC Server.

Importing the configuration file provided as an example, and following the instructions in this section, leads to three tools being made available to users logged into the CLC Server via their Workbench or the Command Line Tools: CLC bio Bowtie Build Index, CLC bio Bowtie List Indices and CLC bio Bowtie Map.

12.7.1 Installing Bowtie

To get started:

- Install Bowtie from <http://bowtie-bio.sourceforge.net/index.shtml>. We assume that Bowtie is installed in `/usr/local/bowtie` but you can just update the paths if it is placed elsewhere.
- Download the scripts and configuration files from <https://resources.qiagenbioinformatics.com/external-applications/bowtie-pp2.zip>
- Place the `clcbio` folder and contents in the Bowtie installation directory. This folder contains the scripts used to wrap the Bowtie functionality. Those wrapper scripts are what is then configured via the External Applications folder.
- Make sure execute permissions are set on these wrapper scripts and on the executable files located in the Bowtie installation directory. The user that will execute these files will be the user that started the CLC Server process.
- Import the `bowtie-pp2.xml` configuration file: Log into the server via the web administrative interface and go to the **External applications**  tab. Expand the "External applications configuration" section and click on the **Import Configuration. . .** button.

The `bowtie-pp2.xml` file contains configurations for three tools associated with Bowtie: CLC Bowtie build index, CLC Bowtie list indices and Bowtie Map. If you already have a set of indices you wish to use and the location of these is known to the system via the `BOWTIE_INDEXES`, then you can just use the Bowtie Map tool via the Workbench and specify the index to use by name.

Otherwise, you can build the index to use using the `CLC Bowtie build index` tool. Here, unless you edit the wrapper scripts in the files you download from CLC bio, the indices will be written to the directory indicated by the `BOWTIE_INDEXES` environmental variable. If you have not specified anything for this, indices will likely be written into the folder called `indexes` in the installation area of Bowtie. Please ensure that your users have appropriate write access to the area indices should be written to.

From ftp://ftp.cbcb.umd.edu/pub/data/bowtie_indexes/ you can download pre-built index files of many model organisms. Download the index files relevant for you and extract them into the `indexes` folder in the Bowtie installation directory.

When configuring Bowtie to run as an external application on master-node setups, the **Environment** configuration will need to be edited. See 12.7.3 for details. In addition, Bowtie indices will have to be placed somewhere accessible to all nodes. One option could be areas configured as Import/Export areas on the *CLC Server*.

The rest of this section focuses on understanding the integration of the `Bowtie Map` tool in particular.

12.7.2 Understanding the Bowtie Map configuration

After the `bowtie-pp2.xml` configuration file has been imported, click the **CLC bio Bowtie Map** name to see the configuration (figure 12.17).

Figure 12.17: The External command tab of the CLC bio Bowtie Map configuration is visible in the external application editor.

From an end-user perspective, when the configuration on the CLC Server is complete, they will be able to launch the CLC bio Bowtie Map tool via their Workbench Toolbox. A wizard will appear, within which they will select the sequencing reads to be mapped, identify the pre-built index file of the reference sequence to use and set a few parameters. The bowtie executable will then be executed on the server system and the results generated will be imported into the CLC Server using post processing tools. The sam mapping file is imported using the Import SAM/BAM Mapping Files tool. A fasta file of sequences mapping to multiple locations is imported using the Fasta High-Throughput Sequencing Import tool.

Below, we step through the General configuration panel and then explain the configuration of the post processing tools that handle the outputs from the bowtie analysis.

General configuration panel

Each of the parameters (items within curly brackets) written into the "Command line" box is presented as an item in the General configuration panel. There, we define the type of information each parameter expects or represents and default values, where relevant.

To understand how these parameters relate to the information that will be passed to the native bowtie executable, please refer to the bowtie_map.sh script in the clcbio folder that should now be in place in the bowtie distribution folder.

Stepping through the parameters in the order they appear in the Command line area of the configuration, and thus the order they appear in the General config panel:

- The `reads` parameter refers to the data that will be provided to bowtie to map. The **User-selected input data** option means the user will be able to select data in a CLC File or Data Location. This data will be exported from the CLC File or Data Location such that the bowtie tool can use it. The second element in this line specifies the format the data should be exported in. This is set to **FASTA (.fa/.fsa/.fasta)** as this is the format the bowtie tool expects sequencing read data.
- The `index` parameter is expecting the name of a bowtie index. Specifying the type **Text** for this parameter means a user will see a box in the Workbench Wizard that they can type text into. Here, a default name, "coli" has been specified, which can be changed by a user launching CLC bio Bowtie Map.

When setting up a tool like this, it would be simpler for users, and much less subject to error, if the type **CSV enum** were selected, and a specified set of indices were listed. Then, a drop down list of options would be provided to the user in a Workbench Wizard, when launching the external application, rather than relying on users typing in the correct names of available bowtie indices.

- The `sam file` parameter refers to the sam mapping file that bowtie will generate as one of its results file. Thus, the type is set to **Output file from CL**. Import of sam files into the CLC Server involves a tool that requires user input. Thus, a post processing tool is configured. This can be seen immediately by the text in the second drop-down box: "Linked with Import SAM/BAM Mapping Files".

If a parameter with type **Output file from CL** is not mapped to a parameter of a post processing step, the text displayed is "Do not standard import / map to high-throughput

sequencing importer". Mapping of outputs to post processing tools is described in more detail below.

The last entry in the configuration of the `sam file` parameter is the name of the sam output file that bowtie should generate. Here it is set to **sam_output**. This file name is used by the bowtie command. The Workbench or Command Line Tools user never sees it.

- The `max number of multimatches` parameter allows a user to select the maximum number of locations a read can map equally well to for it to be included in the mapping. The type is set to **CSV enum**, which means a user will be able to select a value from a drop down list of the 3 values listed in the last field (2,3,4). The first value will be the default. The values in the middle field are those passed to the bowtie wrapper script and then onto bowtie. So, for example, if "2,3,4" were entered in the middle field, and "two, three, four" in the last field, a user could select the option "two", and bowtie would be sent the value 2.
- The `multimatch filename` parameter refers to another output from bowtie, this one containing fasta formatted reads that match to multiple locations of the reference equally well. Since it is a result file, the type is set to **Output file from CL**. We have decided to use a post processing tool to bring the results back into the CLC Server, the Fasta High-Throughput Sequencing Import tool.
- The `max number of mismatches` parameter allows a user to select the maximum number of mismatches to be allowed between a read and the reference in order for a read to be considered as matching the reference at that location. The type is set to **CSV enum**, and is presented to a user in the same way as the `max number of multimatches` parameter described above.
- The `report all matches` option is one that can be turned on or off. Thus it is set to type **Boolean text**. A user will be presented with a checkbox they can select or deselect in the Workbench Wizard. The value in the text field, here "-a", is the one bowtie will be passed if the user selects the checkbox. If the user does not select the checkbox, this parameter will not be sent to bowtie.

Post processing - importing the results from Bowtie

If you expand click on the **High-throughput sequencing import /Post-processing** link below the General configuration area, you will see that there are two post-processing tools selected: the **Import SAM/BAM Mapping Files** tool and the **Fasta High-Throughput Sequencing Import** tool.

In each case, clicking on the **Edit and map paramaters** button below it will bring up the configuration window for that tool. Here, several types of configuration can be carried out.

1. Mapping of outputs of the external application to inputs of the post processing tool.
2. Locking or unlocking of parameters, determining which parameters users can alter when launching the tool via the Workbench or Command Line Tools.
3. Setting default values for parameters of the external application.

Here, we step through the configuration of the **Import SAM/BAM Mapping Files** tool. The configuration of the **Fasta High-Throughput Sequencing Import** is similar.

The parameters in this configuration window are the **Import SAM/BAM Mapping Files** tool parameters, just as would be offered when that tool is launched directly in a CLC Workbench.

A locked lock symbol by a parameter means that the user will not be given access to this option when launching the tool. Default settings for lock parameters are used. The locked parameters shown in figure 12.18 indicate that a track will be output rather than a stand-alone read mapping, unmapped reads will be saved, references will not be downloaded from an external source and, had they been, downloaded references will not be saved. Quality scores and sequence names will be kept (not discarded).

By contrast, the References parameter is unlocked. When using the Import SAM/BAM Mapping Files tool, users need to specify where the relevant reference sequences are. Thus, this option should be made available for users to configure when the tool is being launched.

The input to the Import SAM/BAM Mapping Files also needs to be defined. This is done by mapping the relevant output from the bowtie command to the input parameter for the Import SAM/BAM Mapping Files tool. The output from bowtie is defined by the "sam file" parameter, and the relevant input parameter in the import tool is "Selected files". A drop down list of potentially relevant parameters appears to the left of the "Selected files" parameter. In our example, this has already been mapped to the "sam file" parameter of the command, as shown in figure 12.18.

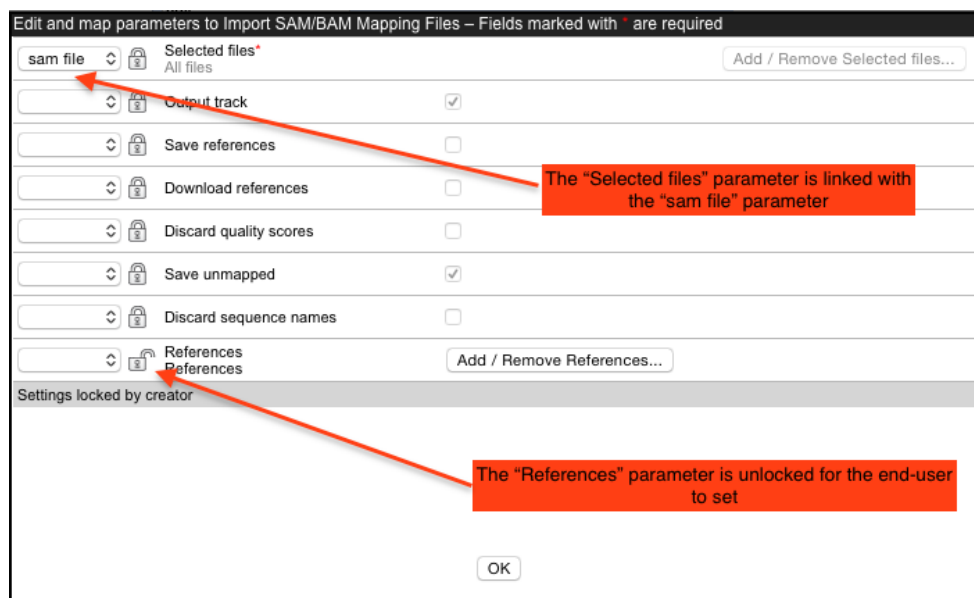


Figure 12.18: Configuration of Import SAM/BAM Mapping Files for import of a sam file after mapping using Bowtie.

Note: The drop-down lists of possibly relevant parameters provided in the post processing tool configuration window are populated based only on the types of parameters (in the General config pane). Any parameters of a type that could be relevant are presented. This means that some parameters appearing in these lists may not make sense contextually.

12.7.3 Setting the path for temporary data

The **Environment** handling shown in figure 12.19 allows you to specify a folder for temporary data and add additional environment variables to be set when running the external application.

Post-processing steps need to access the results files of the external application. Thus, **if you**

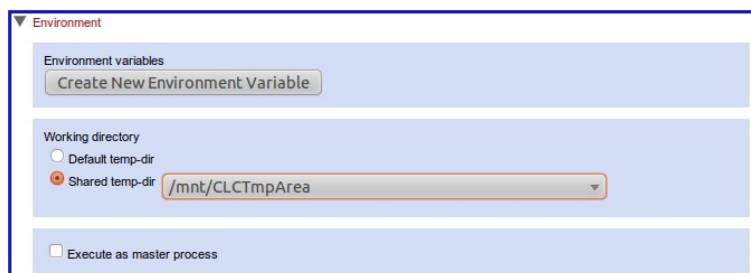


Figure 12.19: Where to save temporary data needs to be defined for Bowtie.

are running on a master-node setup, the directory you choose for these results files must be shared, that is, accessible to all nodes you plan to have as execution nodes for this external application. This is because different stages of your task could be run on different nodes. For example, the export process could run on a different node than the actual execution of the Bowtie script and the post processing. Thus, in a master-node setup, be it using grid or CLC execution nodes, having this shared temporary area eliminates the overhead of transferring the temporary files between nodes.

12.7.4 Tools for building index files

We have also included scripts and configurations for building index files using the external applications on *CLC Server*. This also includes the possibility of listing the index files available. To get these to work, please make sure the path to the Bowtie installation directory is correct.

The Bowtie distribution itself also includes scripts to download index files of various organisms.

12.8 Example: MAFFT (containerized external application)

In this section, we describe how to create a simple containerized external application for MAFFT, a multiple sequence alignment program for amino acid or nucleotide sequences, available from <https://mafft.cbrc.jp/alignment/software/>.

In brief, the steps involved are:

1. Create a Docker image containing MAFFT.
2. Test the Docker image.
3. Upload the Docker image to a repository, such as Amazon Elastic Container Repository (AWS ECR) or DockerHub. (Optional)
4. Configure a containerized external application, making MAFFT available for users of the *CLC Server*.

We assume here that the containerized execution environment for the *CLC Server* has been enabled and configured, as described in section 12.1.1. We also assume that docker has been set up on your local system, and that the account being used to set up docker images and test them, as well as the user running the *CLC Server* process, have permission to run docker.

12.8.1 Create the Docker image

To create a Docker image containing MAFFT, we will create a Dockerfile describing the steps needed to build this image from a base image.

In a text file named "Dockerfile" (without any file extension), enter the following:

```
FROM ubuntu:16.04
MAINTAINER user@domain.com
RUN apt-get update
RUN apt-get install -y wget
RUN mkdir mafft-bin
RUN wget -O /mafft-bin/mafft.tgz https://mafft.cbrc.jp/alignment/software/mafft-7.450-linux.tgz
RUN tar xfvz /mafft-bin/mafft.tgz
```

These statements indicate that the image is to be built on top of Ubuntu 16.04, with the creator's identity specified in the MAINTAINER field. The RUN statements state that wget should be installed, and the MAFFT binary should be downloaded from a public archive and unpacked into a local folder called "/mafft-linux64/" in the Docker container.

An executable called "mafft.bat" is located in the /mafft-linux64/, and it is this executable that we will be using in our external application.

A local docker image can now be built using the Dockerfile and the `docker build` command. From the directory containing the Dockerfile, run the following command:

```
docker build . -t example/mafft:0.0.1
```

When the above command is run, the Ubuntu image is retrieved if it is not already present, and the RUN steps in the Dockerfile are performed. An image is created with the name "example/mafft" and the tag "0.0.1".

Before we configure the external application, we will step through testing our Docker image and (optionally), uploading the image to DockerHub.

12.8.2 Test the Docker image locally

We can now use the docker image just created to run MAFFT locally in a Docker container.

At its simplest, a command like the following can be run, leading to the MAFFT help information being displayed:

```
docker run example/mafft:0.0.1 /mafft-linux64/mafft.bat --help
```

To generate an alignment, we need to supply a FASTA format file as input to MAFFT. This data file must be placed in an area visible to both the host system and the container. In this example, we will be using the `docker -v` command to bind mount a local directory to a container location.

We will put a FASTA format file containing sequences to align, called `sequences.fa` into a local folder called `/home/user1/dockersharearea/`. To run a container with MAFFT, to align this set of sequences, we would run:

```
docker run -v /home/user1/dockersharearea:/mnt/mafft
example/mafft:0.0.1 /mafft-linux64/mafft.bat /mnt/mafft/sequences.fa
```

This command includes the `-v` option with values specifying that the local directory `/home/user1/dockersharearea/` should be bind mounted to `/mnt/mafft` in the container. The final option specifies and where the input data will be found within the container.

The progress of the job is reported to the console, as is the alignment generated.

After successfully testing the image, you can proceed to configure a containerized external application, as described in section section 12.8.4. Optionally, you can also upload the image to a repository, such as Amazon Elastic Container Repository (AWS ECR) or DockerHub at this point, as described in section section 12.8.3 and then use that image in your external application rather than a local one.

12.8.3 Upload the Docker image to a repository

Optionally, the Docker image can be uploaded to a central repository, such as Amazon Elastic Container Repository (AWS ECR) or Docker Hub. In this example, we will upload the image to Docker Hub.

Note: To run workflows containing external applications on the *CLC Genomics Cloud Engine*, the Docker image must be published in the Amazon Elastic Container Repository (ECR) on the same Amazon account where the CLC Genomics Cloud Engine is deployed, as described in the *Cloud Plugin* manual: https://resources.qiagenbioinformatics.com/manuals/cloudplugin/current/index.php?manual=External_applications_in_cloud.html

Log in to Docker Hub:

```
docker login --username=dockerhubusername
```

Find the image ID of the image we just created for MAFFT:

```
docker login --username=dockerhubusername
```

The output should look something like this:

REPOSITORY	TAG	IMAGE ID	CREATED	SIZE
example/mafft	0.0.1	01d5c588523c	2 hours ago	209MB

Take the number in the column "IMAGE ID", and map it to the desired repository on Docker Hub:

```
docker tag 01d5c588523c dockerhubusername/example-repository:0.0.1
```

Finally, push the image to Docker Hub.

```
docker push dockerhubusername/example-repository
```

Before testing the uploaded image works, remove all local images and containers associated with the same ID:

```
docker rmi -f 01d5c588523c
```

Run a command to start up a container created from the image uploaded to DockerHub:

```
docker run -v /home/user1/dockersharearea:/mnt/mafft
dockerhubusername/example-repository:0.0.1 /mafft-linux64/mafft.bat
/mnt/mafft/sequences.fa
```

The initial output will report "Unable to find image 'dockerhubusername/example-repository:0.0.1' locally". The image is then pulled dynamically from the online repository.

12.8.4 Configure a containerized MAFFT external application

In this section, we focus on how to determine the command to be configured for an individual containerized external application, and then step through configuring an external application for the Docker container containing MAFFT.

We assume that the containerized execution environment has already been enabled and configured, as described in section 12.1.1.

Determining the containerized external application command line

When configuring containerized external applications, only the part of the docker command *specific to this particular application* is included in the *Command line* field of the external application configuration. Parts of the command general to running all containerized external applications are specified in the *Containerized execution environment* area, as described in section 12.1.1.

The full command we want to run takes this form:

```
docker run -v <import-export-dir>:<mount-point-in-image> \  
<image-identifier> <command-to-run-from-image> <input-data>
```

With default settings for the containerized execution environment, the first part,

```
docker run -v <import-export-dir>:<mount-point-in-image>
```

is already defined for every containerized external application.

Thus, only the rest of the command needs to be specified when configuring the individual external application, i.e.

```
<image-identifier> <command-to-run-from-image> <input-data>
```

For our MAFFT example, that command would have the form:

```
example/mafft:0.0.1 /mafft-linux64/mafft.bat <inputdata>
```

How to specify this command, including how to specify that users should be able to select the data to be aligned when they launch the tool, is described in detail below.

Settings under the External command tab

To create a new external application, click on the **New configuration...** button under the External Applications Configurations section in the *CLC Server* web administrative interface.

We focus on settings under the "External command" and "Stream handling" tabs in the window that appears.

Configure the following under the **External command** tab:

- In the **External application name** field, type "MAFFT".

Reminder: This name is displayed in the *CLC Workbench* Toolbox menu when the external application is made available for use. It is also the name used for the corresponding workflow element and it forms the basis of the name used for launching the external application using the *CLC Server Command Line Tools*.

- In the **Command line** field, type the following, where the parameter value to be substituted at runtime is indicated by typing its name inside *{curly brackets}*.

```
example/mafft:0.0.1 /mafft-linux64/mafft.bat {Sequences to align}
```

The text inside the curly brackets, here "Sequences to align" will be the label on the input field in the wizard that *CLC Workbench* users see when they launch the MAFFT external application, as shown in figure 12.25. It also forms the basis of a command line parameter when using the *CLC Server Command Line Tools*.

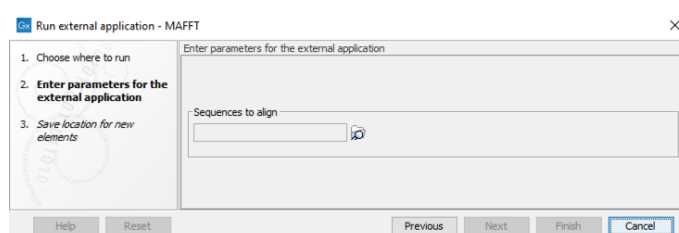


Figure 12.20: The external application name is presented as the name of the corresponding workflow element. Output channels and elements connected to them also reflect names specified in the external application configuration.

When a parameter is written into the *Command line* field in curly brackets, that parameter will be listed in the **General configuration** area below. There, the type of value expected for this parameter is configured.

We want users to select data to be aligned from a CLC location, and as MAFFT accepts data in FASTA format, we need to specify that the selected data should be exported in that format, so:

- In the *Sequences to align* section of the **General configuration** area, select "User-selected input data (CLC data location)" in the first drop-down menu, and select the exporter: "FASTA (.fa/.fsa/.fasta)" from the second drop-down menu.

The exported file will be placed in the shared working directory configured for the containerized execution environment of the *CLC Server*, and the path to this exported file will be substituted into the docker command at runtime.

We now specify that the external application is containerized:

- For the **External application type**, select the option "Containerized: Docker".

Figure 12.21 shows the configuration window after the above steps have been taken.

Figure 12.21: Defining the MAFFT containerized external application: setting up the command.

Settings under the Stream handling tab

The MAFFT application produces its output on standard out and standard error, so we configure the result handling under the **Stream handling** tab, as shown in figure 12.22.

- MAFFT reports alignments in FASTA format to standard out, so in the **Standard out handling** drop-down menu, select the option: "FASTA Alignment (.fa/.fsa/.fasta)" option, which specifies the *CLC Server* importer to use.
In the **File name** field, enter "MAFFT-alignment.fa".
- In the **Standard error handling** section, select the option: "Do not stop execution or show error dialogs".
In left hand, drop-down menu, select the importer: "Plain text (.txt/.text)", and in the **File name** field, enter "MAFFT-log.txt".
MAFFT reports the progress of the alignment to standard error, and docker reports any problems here also. Thus this information can be useful for troubleshooting.

The file names specified for collecting information sent to standard out and standard error are used for the raw files that capture the contents of these streams, and their base names are seen by end users, as illustrated in 12.23 and 12.24 for this external application.

Save the external application

Click on the **Save** button at the bottom of the editor. By default, the external application will now be available directly under the "External Applications" menu of any *CLC Workbench* logged into this *CLC Server*.

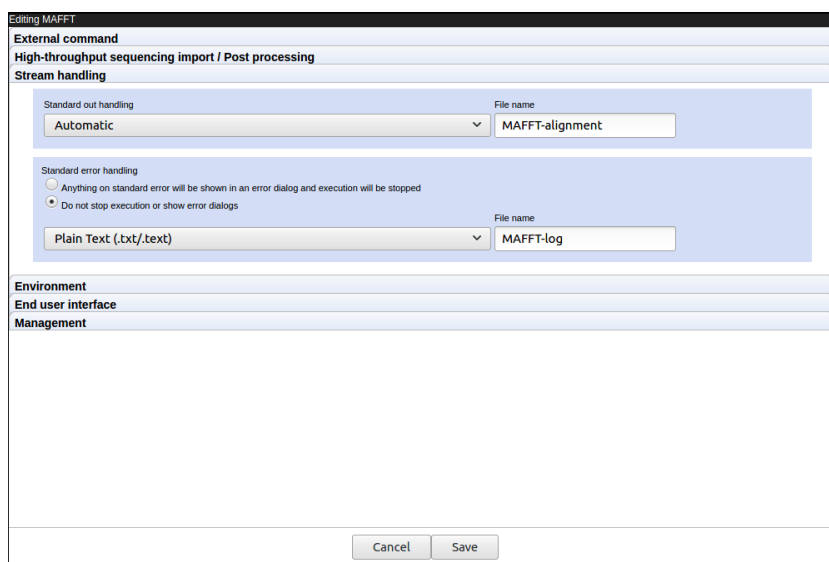


Figure 12.22: Defining the MAFFT containerized external application: output handling.

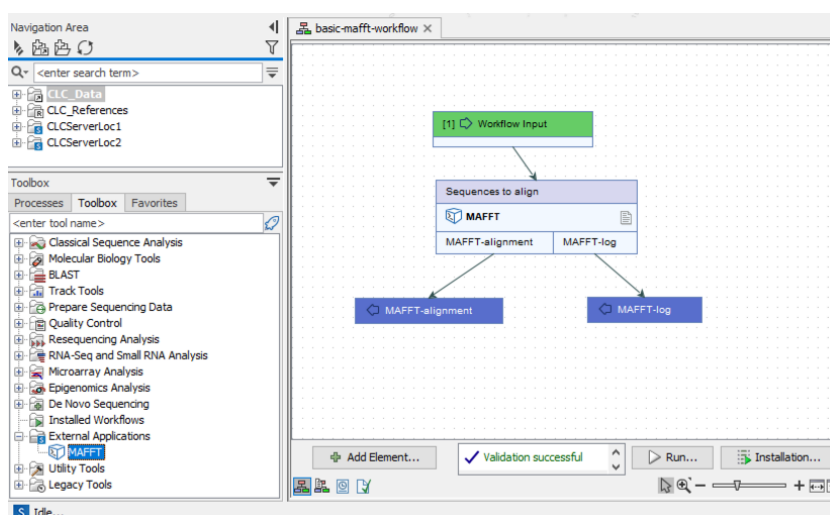


Figure 12.23: The names entered in the external application configuration are used as the name of the corresponding workflow element, the names of the output channels and input channels, and the default names of output elements attached to the output channels.

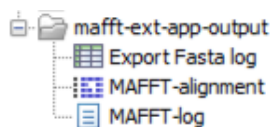


Figure 12.24: The external application was configured to generate output files named "MAFFT-alignment.fa" and "MAFFT-log.txt", which were then imported into the **CLC Server**, where those names are then reflected in the names of the imported data elements.

If you want the external application to be listed in subfolder instead, go to the **End user interface** tab of the editor and specify a subfolder name there.

The configuration is now at a point where we can test this external application from a *CLC Workbench* or the *CLC Server Command Line Tools*. See section 12.2 for further information about configuring external applications.

Launching the MAFFT external application from a CLC Workbench

From a *CLC Workbench* logged into the *CLC Server*, launch the external application directly by going to:

Toolbox | External Applications (📁) | MAFFT (📁)

A wizard should appear. When you get to the step labeled "Enter parameters for the external application", you should see a field labeled "Sequences to align" (figure 12.25), reflecting the name given to that parameter in the external application command configuration.

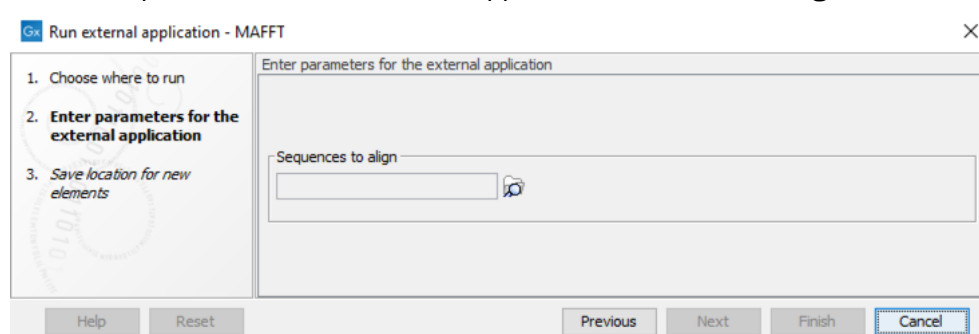


Figure 12.25: The Workbench user sees an option in the wizard named "Sequences to align". That label is taken from the external application command configuration.

To create a workflow that includes the MAFFT external application, open the Workflow Editor of a *CLC Workbench* logged into the *CLC Server*. The MAFFT element should be available to add from dialog that opens when you click on the "Add Element" button.

If the external application configuration has been exported to S3 from a *CLC Server* with the *Cloud Server Plugin* installed, then a *CLC Workbench* with the *Cloud Plugin* can also be used. See section 12.4 for further information about this aspect.

Note: To run external applications on a *CLC Genomics Cloud Engine*, they must be included in a workflow, and then that workflow submitted. To submit jobs to a *CLC Genomics Cloud Engine* from the *CLC Server*, it must have the *Cloud Server Plugin* installed. If submitting the workflow from a *CLC Workbench*, it must have the *Cloud Plugin* installed.

12.9 External applications in workflows

Like most other tools available for execution on the *CLC Server*, tools configured as external applications can be included in workflows.

The inputs and outputs are as configured in the external application itself. In figure 12.26, the external application, CLC bio Bowtie Map is used as a workflow element. In this particular case, the configuration had a single post processing step, the Import SAM/BAM Mapping Files tool. That tool can output a stand-alone read mapping or a read mapping track, and outputs a sequence list containing unmapped reads. Thus these are the output options you see in the workflow element.

Parameters that are locked in the configuration of a workflow element are not offered to the user for editing when the workflow is launched. Parameters that are unlocked are.

Note: External applications can only be used in a workflow if they are configured with at least one "User-selected input data" and at least one import of the data generated. If the external

application does not generate data that is suitable for import then importing the output from standard out or standard error as plain text is recommended. In general it is recommended to always import standard error to help identify potential problems with an external application.

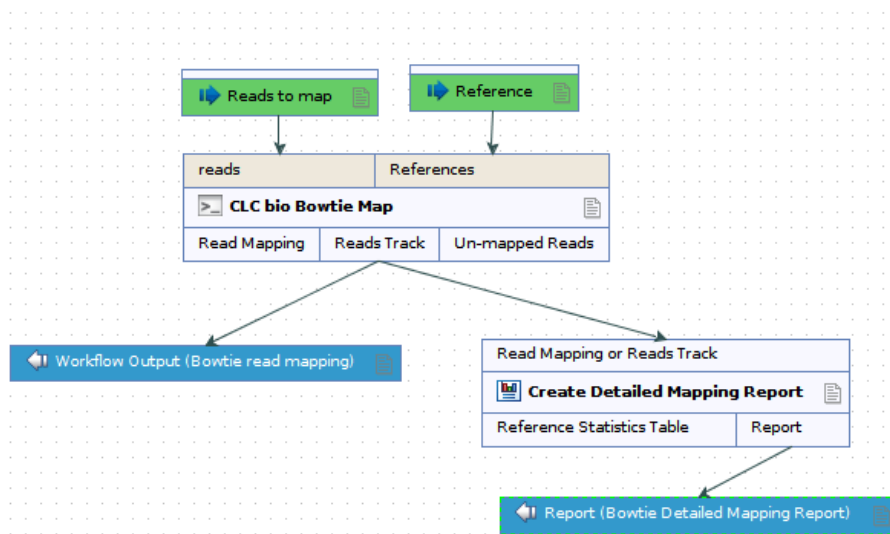


Figure 12.26: The CLC bio Bowtie Map external application used as an element in a workflow. Here, the outputs visible are those provided by the (single) post processing tool configured: Import SAM/BAM Mapping Files

When additional post processing tools are configured, their outputs will be added to those available in the workflow element. See figure 12.27, where a workflow element for the external application, CLC bio Bowtie Map is present, but in this case, the configuration specified two post processing tools: the Import SAM/BAM Mapping Files tool and the Fasta High-Throughput Sequencing Import tool. As earlier, the three outputs associated with the Import SAM/BAM Mapping Files tool are present. In addition, the output from the Fasta High-Throughput Sequencing Import tool, "Imported reads" is present.

The output channel names make sense for individual tools, but may not make sense in the context of a given external application. For example "Imported Reads" makes sense when you run the Fasta High-Throughput Sequencing Import tool by itself. However, in the context of the CLC bio Bowtie Map external application, it is not indicative of what is really being output. Meaningful names can be configured for workflow output elements. See for example figure 12.27, where the output from the Fasta High-Throughput Sequencing Import tool, "Imported reads", has had "bowtie multimapped reads" appended to the name.

For more details about designing and running workflows, see <http://resources.qiagenbioinformatics.com/manuals/clcgenomicsworkbench/current/index.php?manual=Workflows.html>.

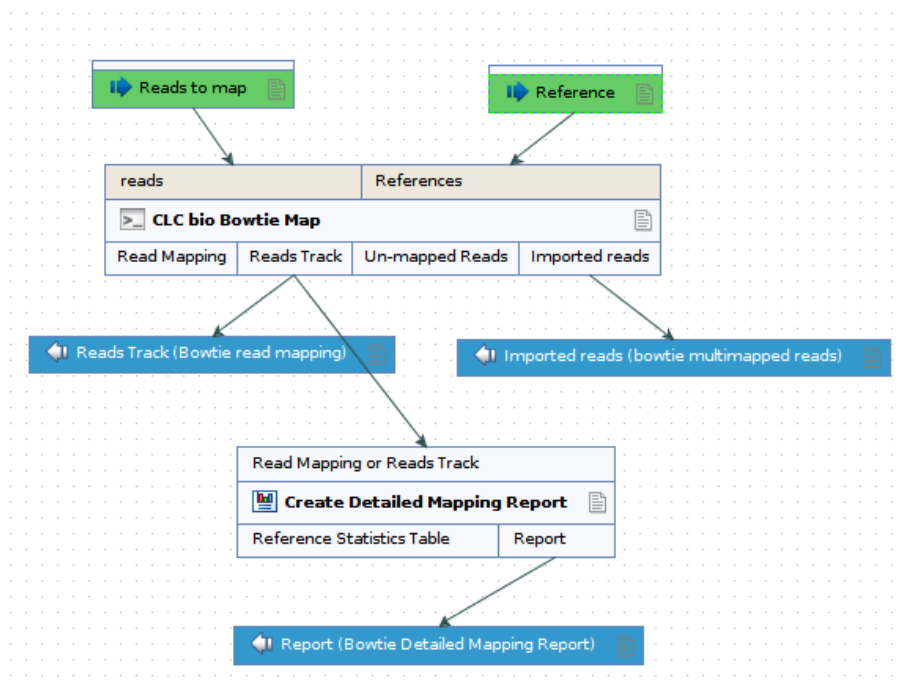


Figure 12.27: The CLC bio Bowtie Map external application used as an element in a workflow. Here, the outputs visible are those provided by the post processing tools configured: Import SAM/BAM Mapping Files and Fasta High-Throughput Sequencing Import.

12.10 Running external applications

External applications can be executed using a *CLC Workbench* or using the *CLC Server Command Line Tools*.

12.10.1 Using a CLC Workbench to launch external applications

Launching external applications from the Toolbox

After connecting to a *CLC Server* with external applications configured and available to client systems, external applications can be executed by going to:

Toolbox | External Applications (📁)

External applications are listed as individual tools in the Toolbox, as shown in figure 12.28. Depending on how they were configured, they may be located within subfolders of the External Applications folder.

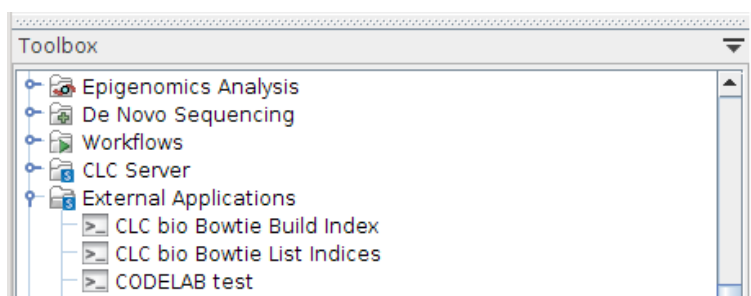


Figure 12.28: Selecting the external application to run.

When an external application is launched, the dialog shown in figure 12.29 is displayed. Depending on your setup, there may be other execution environment to choose from. For example, grid presets will be shown if they have been configured as described in section 6.3.

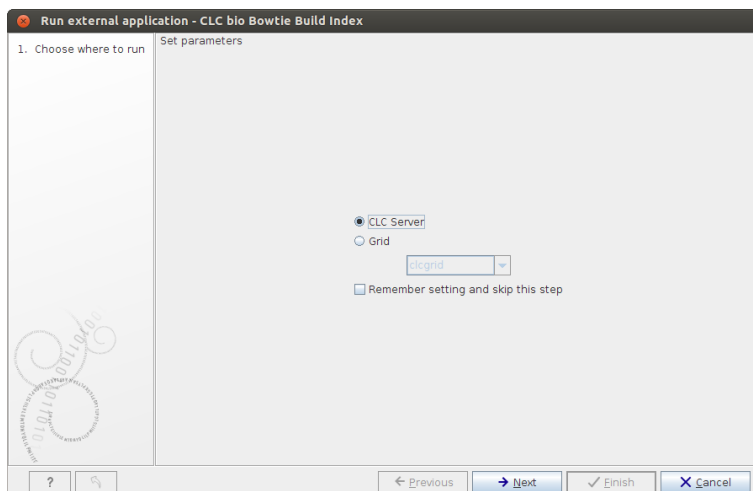


Figure 12.29: Selecting execution environment.

Progress through wizard steps, configuring any settings necessary (figure 12.30).

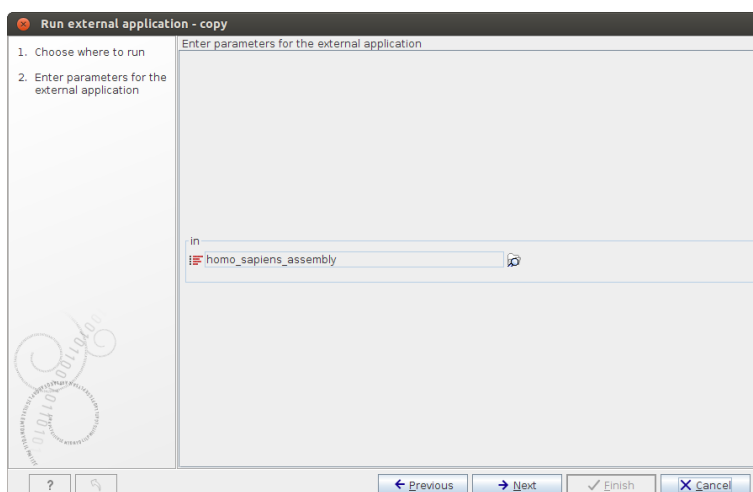


Figure 12.30: Configurable parameters of an external application are presented in the wizard. Here, a sequence list has been selected for the "in" parameter.

Launching external applications as part of a workflow

External applications can be included in workflows, as described in section 12.9. Workflows stored in the Navigation Area can be launched from within the Workflow Editor and installed workflows can be launched from the Workbench Toolbox.

Note: Workflows containing external application elements must be run on a setup where the external application is available. This will either be a CLC Server, a system the CLC Server can launch jobs on, or a CLC Genomics Cloud Engine. Workflows containing external application elements *cannot* be run directly on the CLC Workbench.

12.10.2 Using CLC Server Command Line Tools to launch external applications

The CLC Server Command Line Tools can be used to launch CLC tools, workflows and external applications, directly or within a workflow context, on a *CLC Server*. General information about using the *CLC Server Command Line Tools* can be found in the manual for that software: <https://digitalinsights.qiagen.com/technical-support/manuals/>.

When launching an external application, the CLC Server execution context will be used unless another execution environment is specified. For example, by adding the `-G` option, a grid preset can be specified.

Running a *CLC Server Command Line Tools* command with missing or invalid parameters results in messages about the problem being returned. For example, trying to invoke the *copy* external application described earlier in this chapter with no arguments yields the output below. The final line makes clear the problem: the `-d` and `-in` parameters need to be specified in the command for the job to be executed.

```
clcserver -S <HOSTNAME> -U <USER> -W <PASSWORD> -A copy
Message: Trying to log on to server
Message: Login successful
The following options are available through the command line and the types are as follows:
```

Type	Valid input
-----	-----
<Integer>	A decimal number in the range
[-2147483648;2147483647]	
Example: 42	
<Boolean>	The string true or false
Example: true	
<String>	Any valid string. It is recommended
to enclose all strings in '' to	
avoid issues with the shell	
misinterpreting spaces or double	
quotes	
Example: 'text="My text"'	
<ClcFileUrl>	A valid path to a file on the server
or in the local file system	
Example: clc://serverfile/tmp/export	
<ClcObjectUrl>	A valid path to a Clc object on the
server or locally	
Example: clc://server/pstore1/Variant1	
Option	Description
-----	-----
-A <Command>	Command currently set to 'copy'
-C <Integer>	Specify column width of help output.
-D <Boolean>	Enable debug mode (default: false)
-G <Grid preset names>	Specify to execute on grid.
-H	Display general help.
-O <File>	Output file.
-P <Integer>	Server port number. (default: 7777)
-Q <Boolean>	Quiet mode. No progress output.
(default: false)	
-S <String>	Server hostname or IP-address of the
CLC Server.	
-U <String>	Valid username for logging on to the
CLC Server	
-V	Display version.
-W <String>	Clear text password or domain
specific password token.	
-d, --destination <ClcServerObjectUrl>	Destination for import from External
Application	
--in <ClcServerObjectUrl>	Model object(s) to be exported to
FASTA (.fa/.fsa/.fasta)	
Error: Missing required options: d, in	

12.11 Troubleshooting external applications

There is no check for the consistency of the external application configuration when it is set up. If there are problems, these will first be seen by the end user, when the application is executed. For example, in a *CLC Workbench*, summary information will shown in a dialog. This may help to identify the issue. If this summary information does not help, try opening the **Advanced** tab, where an extended error message should be visible.

Below are some tips to aid with troubleshooting issues with external applications.

- Configure the external application to import standard out and/or standard error as text. This makes it possible to check error messages posted by the external application. See figure 12.31. For containerized external applications, messages from docker are posted to standard error, so collecting standard error for such applications is particularly recommended.

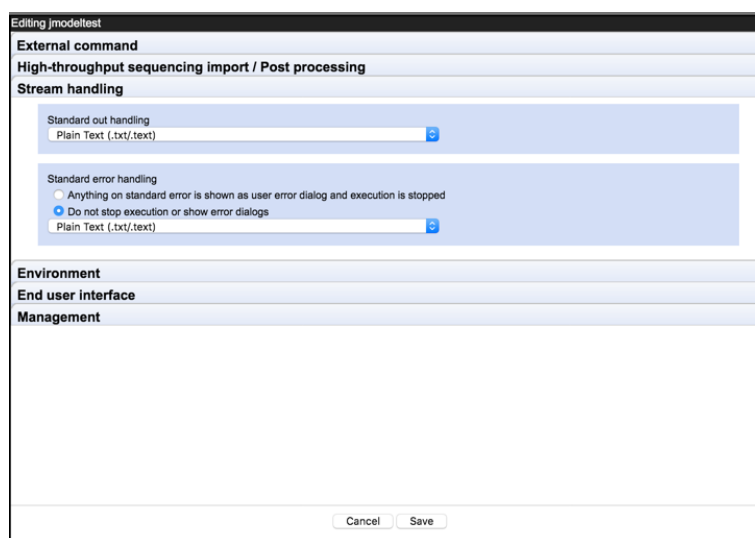


Figure 12.31: Standard error and standard out from the command line application can be collected and imported so it can be reviewed.

- If your external application was previously working and then stops working, check if the configuration was recently changed. Each time a change is made the version number of the external application is updated. The name of the user who made the most recent change in the listing under the **External application configurations** area, and also under the **Management** tab of the editor for each individual external application. Only users with admin privileges are able to edit external applications configurations.
- Check the third party application/container can be run:
 - For standard external applications:
 - * Is the application being found? Check that the path to the application is complete and correct.
 - * Is the application executable, and can it be executed by the user running the *CLC Server* process?
 - * If there is a wrapper script calling the third party application, does it contain the correct path to the application? Is the wrapper script executable?

- For containerized external applications:
 - * Does the user running the *CLC Server* have permission to run Docker? (Is that user a member of the docker group?)
 - * Is the reference to the container in the Command line field of the external application configuration valid?
 - * Is the *CLC Server* running on a Windows system? Containerized external applications are only supported for Linux-based setups.
- Check the import/export directory configurations, where relevant.
 - For standard external applications, the default temp dir is used by default for temporary files, but an import/export directory may be specified for this purpose instead, as described in section 12.2.5. If this has been done, check the import/export directory is available and is writable by the user running the *CLC Server* process.
 - For containerized external applications, an import/export directory is specified as the shared working directory in the containerized execution environment settings, as described in section 12.1.1. Besides being available and writable by the user running the *CLC Server* process, the selected directory must be shareable between the host system and containers.
- Check for conflicts in the naming of the external application.

If your users will only access external applications via a *CLC Workbench*, then you do not have to worry about what name you choose when setting up the configuration. However, if they plan to use the *CLC Server Command Line Tools*, to interact with your *CLC Server*, then please ensure that you do not use the same name as any of the *CLC Server* internal commands. You can get a list of these by running the `clcservice` command, with your *CLC Server* details and no tool specified. I.e. a command of the form:

```
clcservice -S <host> -P <port> -U <username> -W <password or token>
```

Chapter 13

Workflows

A workflow consists of a series of tools where the output of one tool is connected as the input to another tool. A workflow created using a CLC Workbench can be run on a *CLC Server* when all the tools in the workflow are available on the server, and the workflow is:

- **Stored in a CLC File Location**, and then opened from the Navigation Area of a CLC Workbench logged into the server and run from the Workflow Editor.
- **Installed on a CLC Workbench** that is logged into the server. When launching, the user can choose to run the workflow on the CLC Workbench or *CLC Server*.
- **Installed on a CLC Server**. Such workflows can be launched from a CLC Workbench logged into the server. When launching, the user can choose to run the workflow on the CLC Workbench or *CLC Server*. These workflows can also be launched using the *CLC Server Command Line Tools*.

A benefit of installing workflows on the *CLC Server* is that it allows control over the version of a workflow being used, as well as easy deployment of new versions when desired. Changes made to such centrally installed workflows become immediately available for all CLC Workbench users logged into the server.

This chapter focuses on server-specific aspects of workflows. General information about workflows are available at: <http://resources.qiagenbioinformatics.com/manuals/clcgenomicsworkbench/current/index.php?manual=Workflows.html>.

13.1 Installing and configuring workflows

After a workflow is created in a CLC Workbench, an installer file can be created, as described on http://resources.qiagenbioinformatics.com/manuals/clcgenomicsworkbench/current/index.php?manual=Creating_workflow_installation_file.html.

Workflow installer files can be used to install the workflow on other CLC Workbenches or on the *CLC Server*. When logged into the *CLC Server* from a Workbench as a user with administrative rights, workflows can also be installed on the server directly from the CLC Workbench.

When working logged into the *CLC Server* web interface as an administrative user, workflows can be installed by going to:

Admin (⚙️) | Workflows (📁)

Click the **Install Workflow** button and select a workflow installer file.

Once installed, a validated (✅) or attention (⚠️) status icon will be shown to the left of the workflow name, as shown in figure 13.1.

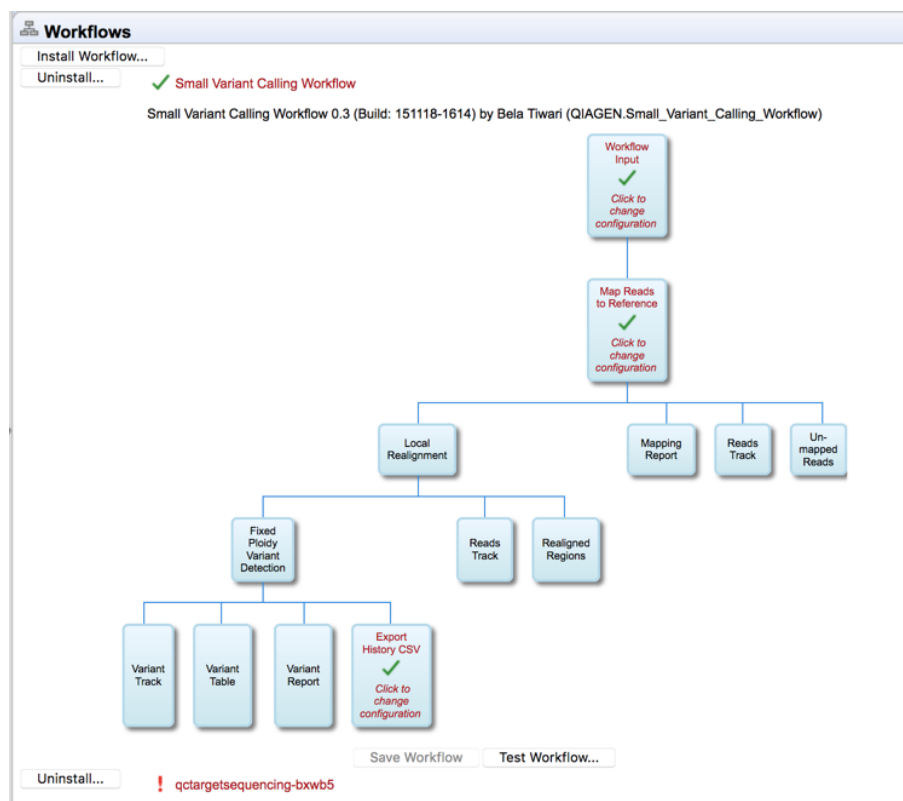


Figure 13.1: The workflow named *Small Variant Calling Workflow* is installed on the server and has been validated. The workflow below, named *qctargetsequencing-bxwb5* is installed, but there are issues that need to be addressed, as indicated by the red exclamation mark.

The workflow elements with red text are ones that can be configured. Click on such an element to bring up a dialog with a listing the parameters that can be configured, as well as an overview of the locked parameters. An example is shown in figure 13.2.

Open parameters can be configured, and can also be locked if desired, so that the parameter cannot be changed when executing the workflow. Locking and unlocking parameters is described further here: http://resources.qiagenbioinformatics.com/manuals/clcgenomicsworkbench/current/index.php?manual=Locking_unlocking_parameters.html.

If changes to the parameter settings of an installed workflow are made, the timestamp of the most recent change and the name of the administrator who made those changes are reported at the top of the workflow configuration view.

Figure 13.2: In this example only one parameter can be configured, the rest of the parameters are locked for the user.

13.2 Executing workflows

Execution of workflows on a server setup

How workflows are run on a multi-node server setup depends on options configured under the **Job Distribution** tab of the web administrative interface. This is described in section 6.7, including outlining key considerations when choosing the most efficient option for a particular setup.

A user perspective on executing workflows

When you log in on the server using a CLC Workbench, workflows installed on the server automatically become available in the **Installed Workflows** folder of the **Toolbox**, as shown in figure 13.3.

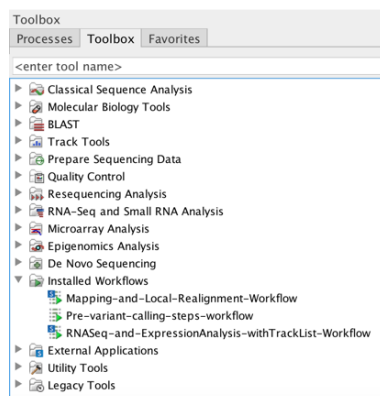


Figure 13.3: Two workflows are installed on the **CLC Server**, as signified by the blue S in their icons. The other installed workflow is installed locally, on the Workbench.

Wherever the workflow is located, when it is launched to run from a CLC Workbench, the user will be presented with a dialog with options of where to run it, as shown in figure 13.4.

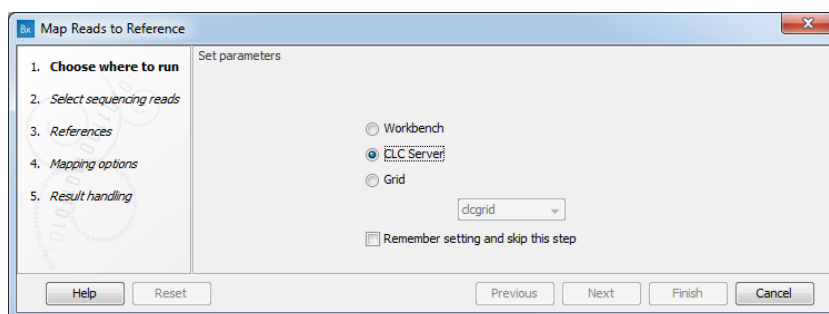


Figure 13.4: Selecting where to run the workflow.

13.3 Updating workflows

Tools included in a workflow are versioned. They will initially be the same version as in the software that was used to design the workflow. If one or more tools are updated through upgrading the *CLC Server* or plugins installed on it, then any workflow containing one or more such tools must be updated.

An exclamation mark (!) is presented beside any workflow that needs to be updated. Clicking on the workflow name opens up a view where each element that needs to be updated is also indicated with an exclamation mark. See figure 13.5. Workflows that can be updated directly in the web administrative interface will have a button at the bottom labeled "Update Workflow" enabled. For workflows that cannot be updated this way, a message will appear stating this, and providing some tips of how to proceed. Details of both these situations are outlined below.

Updating workflows via the server web administrative interface

A button labeled "Update Workflow" just under the workflow is enabled for workflows that can be updated directly in the web administrative interface. Clicking on this button, or any of the elements with exclamation marks, starts the update. See figure 13.5.

Note! If a tool has been updated with a new parameter, then an updated workflow that includes that tool will have that new parameter configured with the default value.

When updating, a window appears containing information about the changes to be enacted if you proceed. If errors have occurred these will also be displayed. See figure 13.6. Accept the changes by pressing the "Update" button. The update can also be canceled at this point if desired.

After pressing the "Update" button, the updated workflow will be marked with a green check mark (✓). A copy of the original workflow is also kept. It is disabled and has the original name with "-backup (disabled)" appended. An example is shown in figure 13.7.

If you click on the copy of the original workflow, a button labeled "Re-enable Workflow" appears (figure 13.8). Clicking on this button re-enables the original workflow and uninstalls the updated version of the workflow.

Updating workflows that cannot be updated via the server web administrative interface

Some installed workflows cannot be updated directly in the web administrative client. Common situations where this can occur include:

1. Workflows containing tools provided by plugins not installed on the *CLC Server*.

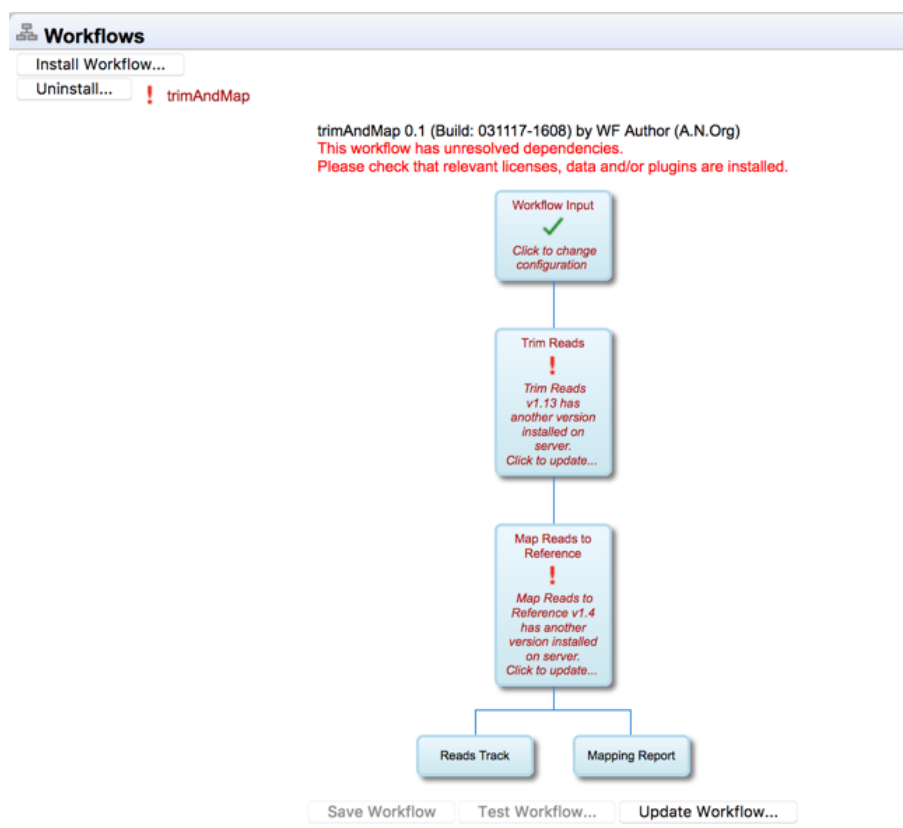


Figure 13.5: Click on the "Update Workflow" button, or on an element marked with an exclamation mark to start the update.

2. Workflows containing tools from server extensions (commercial plugins) that require a license, but either the license is not present or it does not support the version of the server extension that is installed.
3. Workflows containing tools not on the version of the *CLC Server* running.
4. Workflows containing tools that cannot be upgraded directly due to the nature of the changes made to them in the updated *CLC Server*.

To resolve the first 2 circumstances, check install any needed plugins and licenses, restart the *CLC Server*, and check the status of workflows under the **Workflows** tab of the web administrative interface.

To address the third and fourth issues, new versions of the workflows must be made on a *CLC Workbench* and then installed on the *CLC Server*. For this, a *Workbench* version that the installed workflow can be run from is needed, as well as the latest version of the *Workbench*.

Updating installed workflows when using software in a higher major version line

To update an installed workflow after upgrading to software in a higher major version line, you need a copy of the older *Workbench* version, which the installed workflow can be run on, as well as the latest version of the *Workbench*.

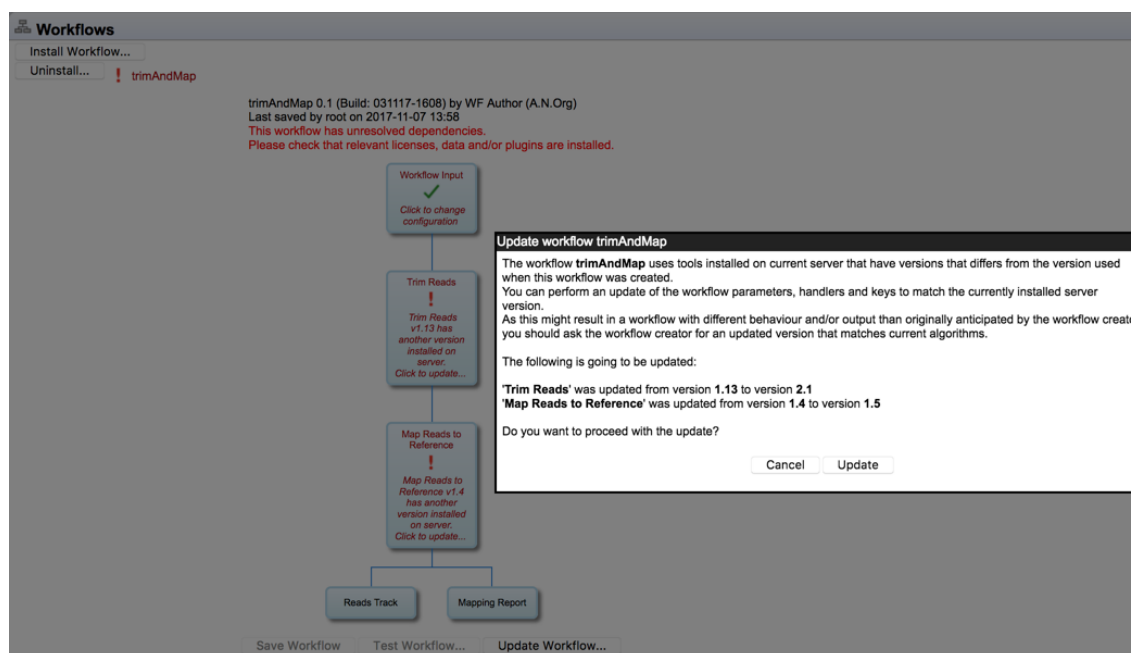


Figure 13.6: Details about the upgrade are presented, and you can choose whether to proceed with the update, or cancel it.

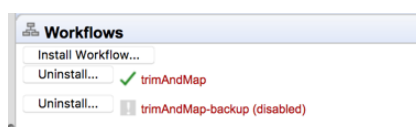


Figure 13.7: In addition to the updated version of the workflow, marked with a green check mark, a copy of the original workflow is kept. It is disabled and has the original name with "-backup (disabled)" appended.

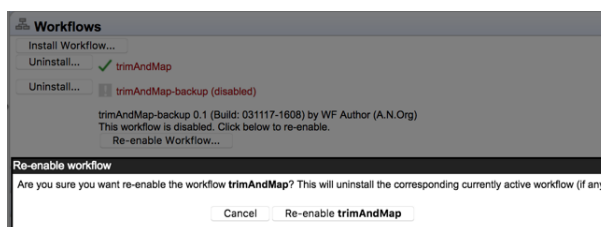


Figure 13.8: After a workflow has been updated, it is possible to re-enable the original workflow.

To start, open a copy of the installed workflow in a version of the Workbench it can be run on. This is done by selecting the workflow in the **Installed Workflows** folder of the **Toolbox** in the bottom left side of the Workbench, then right-clicking on the workflow name and choosing the option "Open Copy of Workflow" (figure 13.9).

Save the copy of the workflow. One way to do this is to drag and drop the tab to the location of your choice in the Navigation Area.

Close the older Workbench and open the new Workbench version. In the new version, open the workflow you just saved. Click on the **OK** button if you are prompted to update the workflow.

After checking that the workflow has been updated correctly, including that any reference data is configured as expected, save the updated workflow. Finally, click the **Installation** button to install the workflow, if desired.

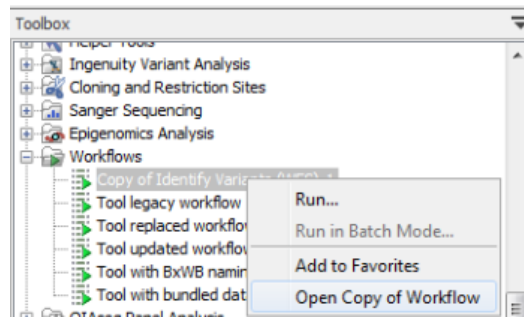


Figure 13.9: Open a copy of an installed workflow by right-clicking on its name in the Workbench Toolbox.

If the above process does not work when upgrading directly from a much older Workbench version, it may be necessary to upgrade step-wise by upgrading the workflow in sequentially higher major versions of the Workbench.

The updated workflow can now be installed on the *CLC Server* as described in section [13.1](#).

Chapter 14

Genomics Analysis Portal

The *Genomics Analysis Portal* is a browser-based, graphical client for the *CLC Server*, offering a controlled environment for processing samples using workflows. Using the *Genomics Analysis Portal*, workflows can be launched using fastq format files as input, their progress can be monitored, and results can be accessed. Options in workflows run using *Genomics Analysis Portal* are locked. Users select input data and the workflow is run using the setting values configured in the installed workflow.

Workflows are made available via *Genomics Analysis Portal* by the administrator by installing them on the *CLC Server* and setting group-level permissions to enable access by relevant sets of users.

Configuring workflows and opening analysis results is done using a *CLC Genomics Workbench* compatible with the version of the *CLC Server* being used.

The *Genomics Analysis Portal* manual is available at

<https://resources.qiagenbioinformatics.com/manuals/genomicsanalysisportal/current/index.php>

The following sections focus on enabling and administering the *Genomics Analysis Portal*.

Enabling the Genomics Analysis Portal

Enabling the *Genomics Analysis Portal* is done under the Extensions tab of the web administrative interface, in the "Genomics Analysis Portal" area. By default, *Genomics Analysis Portal* is not available for use.

Clicking on the **Configure** button opens a dialog where there is an Enable option and fields for entering credentials for a service user (figure 14.1). This user is used for running the workflows launched using the *Genomics Analysis Portal*. Service user details must be provided before the *Genomics Analysis Portal* will be available for users.

Note that the user name and password for the service user can be changed in two places:

1. From the location described here, i.e. Genomics Analysis Portal tab under the Extensions tab of the server web administrative interface.
2. From the **Service user** item in the **Configuration** tile of the *Genomics Analysis Portal* Administration page, visible when you are logged in as root.

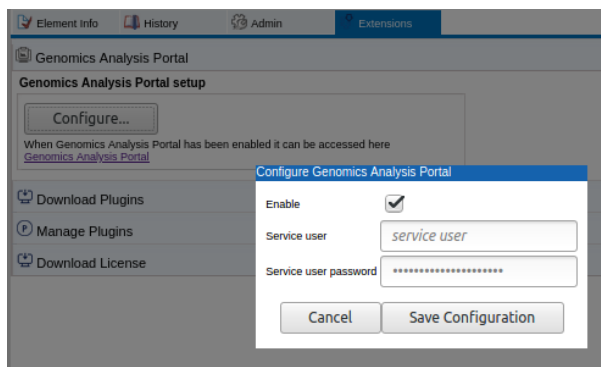


Figure 14.1: Clicking on the *Configure* button opens a dialog for enabling the *Genomics Analysis Portal* and entering service user credentials.

After making changes, the *CLC Server* needs to be restarted. This can be done using functionality offered in the *Status and Management* area under the *Admin* tab, as described in section 7.

Accessing the Genomics Analysis Portal

The URL to the *Genomics Analysis Portal* interface is provided just under the **Configure** button. It takes the form `http://serverURL:7777/gap/`.

Users enter that URL into a web browser and then log into *Genomics Analysis Portal* with their *CLC Server* credentials (figure 14.2).

All *CLC Server* users are able to log into the *Genomics Analysis Portal* once it is enabled, but in the **Start analysis** workflow drop-down menu, they only see workflows they have been authorized to use.

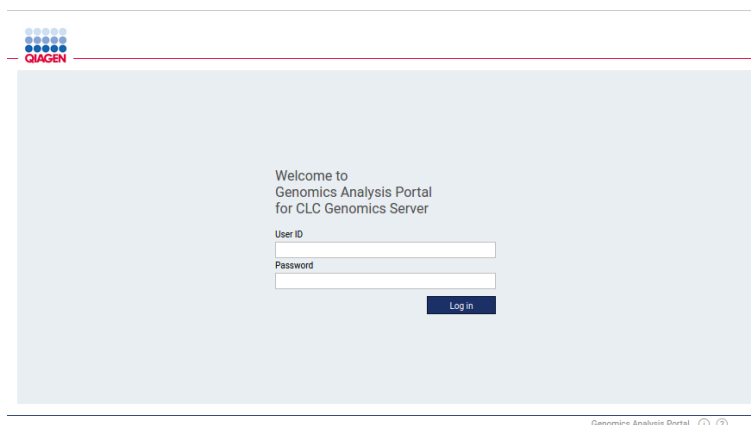


Figure 14.2: Users log into the *Genomics Analysis Portal* using their *CLC Server* credentials.

Authorizing access to workflows via the Genomics Analysis Portal

For a workflow to be available via the *Genomics Analysis Portal*, permissions must be set giving access to it. To do this:

1. Go to **Admin** (🔧) | **Global permissions** | **Workflows**
2. Locate the relevant installed workflow and click on **Edit permissions**.

3. Choose **Only authorized users from selected groups** and select the user group(s) who should have access to that workflow (figure 14.3).

Edit list and execution permissions for DHS-3501Z QIAseq Comprehensive Cancer Panel (Illumina)

Listing and execution of DHS-3501Z QIAseq Comprehensive Cancer Panel (Illumina) is granted to:

All authorized users

Only authorized users from selected groups

Enter search term

admin

GAP

Select all Select none

Save Cancel

Figure 14.3: Installed workflows must be authorized for one or more groups to it be available via the Genomics Analysis Portal.

Chapter 15

Troubleshooting

Various provisions are in place to help support the administration of your *CLC Server*. These include automatic checks for consistency when certain types of configuration changes are made, a tool called "check setup" that can be run at any time from the web administrative interface and that runs automatically when an administrator logs in, and a bug reporting setup. In this chapter, we cover the latter two features.

Troubleshooting tips for specific areas of a server setup can be found in dedicated sections in the manual, including:

- Troubleshooting server startup and permissions on **Linux** is covered in section [2.7.3](#).
- **Grid Integration Tips** are given in section [6.3.13](#).
- Troubleshooting **External Applications** is covered in section [12.11](#).

15.1 Check setup

The **check setup** tool checks your *CLC Server* is set up correctly. The tool is run automatically each time an administrative user logs into the web administrative interface. If issues are found, a red band and a warning message in red will be visible, as shown in figure [15.1](#). Clicking on the warning message will open the report, where details of the problems can be found, as shown in figure [15.2](#).

The **check setup** tool can also be run on demand when logged into the web administrative interface by clicking on the **check setup** link in the top right hand corner and then clicking on the **Generate Diagnostics Report** button in the window that appears.

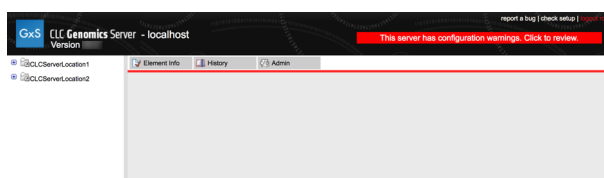


Figure 15.1: If issues with the server configuration have been found, a red band and warning message is presented. Clicking on the warning will open the report.

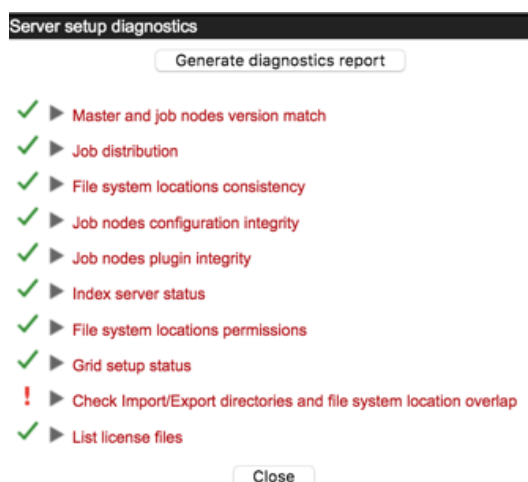


Figure 15.2: Tests that passed are marked with a green check mark. Tests that failed are marked with a red exclamation mark. Here, a problem with the setup of import/export directories has been found.

Any tests where problems were identified are marked with a red exclamation mark. A green check mark is placed beside tests that passed. Click on any of the test names to see further information.

Additional notes:

- A green check mark is presented beside "List license files" when the contents of the "licenses" folder in the installation area of the CLC Server can be listed. Click on this item to see a list of the licenses found and the products and versions supported by those licenses found are reported. Information about expired licenses is also presented. See figure 15.3.
- A green check mark is presented beside "Grid setup status" in two cases:
 - You have configured a grid setup and it is configured correctly.
 - You have not configured a grid setup.

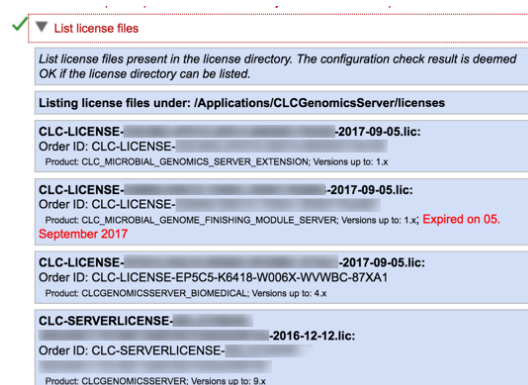


Figure 15.3: Click on the List license files item in the report to see the list of the license files found in the licenses subfolder of the installation area. Products and versions supported are reported, and any expired license is noted with red text.

15.2 Bug reporting

Please contact our Support team if you have problems with the installation and configuration of your *CLC Server*. It can often be helpful if you provide information about the server configuration and the logs directly. To do this, you can submit a bug report from the web administrative interface by clicking on the **report a bug** link in the top right corner. This opens a bug report dialog, as shown in 15.4. Enter the relevant information with as much detail as possible. If the server has access to the internet, click on the **Submit Bug Report** button to send the report directly to QIAGEN Bioinformatics Support. If the server does not have access to the internet, click on **Download bug report** to create a zip file that you can attach to an email you send to ts-bioinformatics@qiagen.com from a machine connected to the network.

Where logs or configuration information are unlikely to be relevant to your questions, please feel free to email the Support team directly at ts-bioinformatics@qiagen.com.

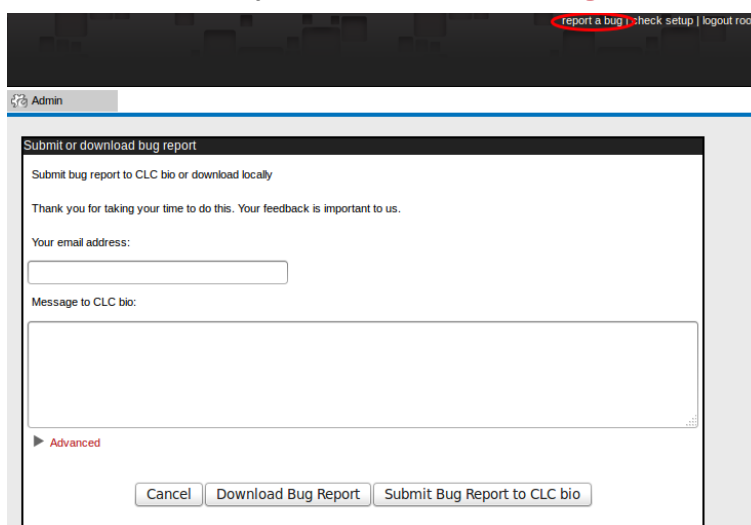


Figure 15.4: Submitting a bug report.

The bug report generated when you click on the **report a bug** link includes the following information:

- *CLC Server* log files
- A subset of the audit log showing the last events that happened on the *CLC Server*
- The *CLC Server* configuration files

No password information is included in the bug report.

In a job node setup you can include the information from the job nodes by checking the **Include comprehensive job node info** checkbox in the **Advanced** part of the dialog.

The process of gathering the information for the bug report can take a while, especially for job node setups.

If a *CLC Workbench* user experiences a server-related error, it is also possible to submit a bug report from a *Workbench* error dialog if they are presented with one. The same archive is included as when submitting a bug report from the server web interface.

All data sent to ts-bioinformatics@qiagen.com is treated confidentially.

Chapter 16

Command line tools

CLC Server Command Line Tools is a command-line client for the *CLC Server*. Installation and basic usage information can be found in the *CLC Server Command Line Tools* manual. Links are provided below. The html version also contains extensive usage information for the commands that can be run.

- **html:** <http://resources.qiagenbioinformatics.com/manuals/clcservercommandlinetools/current/>
- **pdf:** http://resources.qiagenbioinformatics.com/manuals/clcservercommandlinetools/current/User_Manual.pdf

Chapter 17

Appendix

17.1 Use of multi-core computers

The tools listed below can make use of multi-core CPUs. This does not necessarily mean that all available CPU cores are used throughout the analysis, but that these tools benefit from running on computers with multiple CPU cores.

- Amino Acid Changes
- Annotate and Merge Counts (legacy)
- Annotate from Known Variants
- Annotate with Conservation Scores
- Annotate with Exon Numbers
- Annotate with Flanking Sequences

- Basic Variant Detection
- BLAST (will not scale well on many cores)

- Call Methylation Levels
- Compare Sample Variant Tracks (legacy)
- Copy Number Variant Detection
- Create Alignment
- Create RRBS-fragment Track

- Demultiplex Reads
- De Novo Assembly
- Differential Expression
- Differential Expression in Two Groups

- Extract and Count (legacy)

- Filter against Known Variants
- Filter based on Overlap
- Fixed Ploidy Variant Detection

- GO Enrichment Analysis

- Identify Enriched Variants in Case vs Control Samples
- InDels and Structural Variants

- K-mer Based Tree Construction

- Link Variants to 3D Protein Structure
- Local Realignment
- Low Frequency Variant Detection

- Map Bisulfite Reads to Reference
- Map Reads to Contigs
- Map Reads to Reference
- Maximum Likelihood Phylogeny
- Merge Annotation Tracks
- Model Testing

- Predict Splice Site Effect

- QC for Read Mapping
- QC for Sequencing Reads
- QC for Targeted Sequencing

- Remove Variants Present in Control Reads
- Remove Marginal Variants
- Remove Reference Variants (legacy)
- RNA-Seq Analysis

- Trim Reads
- Trio Analysis

17.2 Database configurations

To use an SQL database for data management with the *CLC Server*, the appropriate JDBC driver for your database system must be installed. This is described in section [17.2.1](#).

For MySQL installations, please also refer to section [17.2.2](#) for information specific to MySQL database configuration.

17.2.1 Installing JDBC drivers

The general steps for installing JDBC drivers for use with CLC software are:

1. Download the appropriate JDBC driver for your database system from the provider. Further details about this are provided below.

2. Place the driver into the `userlib` directory in the installation area of the *CLC Server*.
 - For a *CLC* job node setup, the JDBC driver file must be placed into the `userlib` folder under the *CLC Server* installation area on **the master node and also on each of the job nodes**.
 - For a grid node setup, the driver file only needs to be placed into the `userlib` folder of the master *CLC Server* installation area.
3. Restart the *CLC Server* software.
 - For a job node setup, restart the master server and each of the job nodes.
 - For a grid setup, only the master *CLC Server* needs to be restarted. This will cause the changes to be deployed to the grid workers.

Getting JDBC drivers

Information on obtaining JDBC drivers for supported DBMS systems is provided in this section. After obtaining the driver, the general instructions given above should be followed to complete the driver installation.

MySQL JDBC Drivers

1. Go to <http://dev.mysql.com/downloads/connector/j/> to download the driver.
2. Choose the option **Platform Independent** when selecting a platform.
3. After clicking on the button to Download, you can login if you already have an Oracle Web account, or you can just click on the link that says `No thanks, just start my download` further down the page.
4. Uncompress the downloaded file and move the driver file, which will have a name of this form: `mysql-connector-java-X.X.XX-bin.jar`, to the folder called `userlib`, found in the installation area of the *CLC Server*.

PostgreSQL JDBC Drivers

1. Go to <https://jdbc.postgresql.org/download.html> and download the relevant driver.
2. Place it in the folder called `userlib`, found in the installation area of the *CLC Server*.

Microsoft SQL Server

1. Go to <https://docs.microsoft.com/en-us/sql/connect/jdbc/download-microsoft-jdbc-driver-for-sql-server> and download the relevant driver.
2. Follow the installation instructions given for the driver to the point where the downloaded file has been unpacked.
3. Move the driver jar file compatible with java 1.8 to the folder called `userlib`, found in the installation area of the *CLC Server*.

Oracle JDBC Drivers

1. Go to <http://www.oracle.com/technetwork/database/application-development/jdbc/downloads/index.html>.
2. Select the relevant version for your Oracle database version.
You will need an Oracle account to download the driver.
3. Move the driver jar file to the folder called `userlib`, found in the installation area of the *CLC Server*.

17.2.2 Configuring MySQL

We recommend basing your MySQL configuration on the example configuration file `my-large.cnf` included in the MySQL distribution.

In addition the following changes should be made:

- Increase the value of the `max_allowed_packet` setting to support transfer of large binary objects to and from the database will be supported. We recommend this setting:
`max_allowed_packet = 64M`
- Ensure InnoDB is available and configured. This is necessary for the MySQL instance to work properly with the *CLC Server*.
- Enable the options in the InnoDB section of the configuration as outlined below:

```
# You can set .._buffer_pool_size up to 50 - 80 %
# of RAM but beware of setting memory usage too high
innodb_buffer_pool_size = 256M
innodb_additional_mem_pool_size = 20M
# Set .._log_file_size to 25 % of buffer pool size
innodb_log_file_size = 64M
innodb_log_buffer_size = 8M
innodb_flush_log_at_trx_commit = 1
innodb_lock_wait_timeout = 50
```

Additionally, there appears to be a bug in certain versions of MySQL that can cause the cleanup of the query cache to take a very long time. If you experience this, please disable the query log by setting the `query_cache_size` option to 0: `query_cache_size= 0`

17.3 SSL and encryption

The *CLC Server* supports SSL communication between the Server and its clients (i.e. Workbenches or the *CLC Server Command Line Tools*). This is particularly relevant if the server is accessible over the internet as well as on a local network.

The default configuration of the server does not use SSL.

17.3.1 Enabling SSL on the server

A **server certificate** is required before SSL can be enabled on the *CLC Server*. This is usually obtained from a *Certificate Authority* (CA) like Thawte or Verisign (see http://en.wikipedia.org/wiki/Certificate_authorities).

A **signed certificate** in a `pkcs12` keystore file is also needed. The keystore file is either provided by the CA or it can be generated from the private key used to request the certificate and the signed-certificate file from the CA (see section 17.3.1).

Copy the keystore file to the `conf` subdirectory of the *CLC Server* installation folder.

Next, the `server.xml` file in the `conf` subdirectory of the *CLC Server* installation folder has to be edited to enable SSL-connections. Add text like the following text to the `server.xml` file:

```
<Connector port="8443" protocol="HTTP/1.1" SSLEnabled="true"
    maxThreads="150" scheme="https" secure="true"
    clientAuth="false" sslProtocol="TLS"
    keystoreFile="conf/keystore.pkcs12" keystorePass="tomcat"
    keystoreType="PKCS12"
/>
```

Replace `keystore.pkcs12` with the name of your keystore file, and replace `tomcat` with the password for your keystore.

The above settings make SSL available on port 8443. The standard (non-SSL) port would still be 7777, or whatever port number you have configured it to.

Self-signed certificates can be generated if only connection encryption is needed. See http://www.akadia.com/services/ssh_test_certificate.html for further details.

Creating a PKCS12 keystore file

If the certificate is not supplied in a `pkcs12` keystore file, it can be put into one by combining the private key and the signed certificate obtained from the CA by using `openssl`:

```
openssl pkcs12 -export -out keystore.pkcs12 -inkey private.key -in certificate.crt -name "tomcat"
```

This will take the private key from the file `private.key` and the signed certificate from `certificate.crt` and generate a `pkcs12`-store in the `keystore.pkcs12` file.

17.3.2 Logging in using SSL from the Workbench

When the Workbench connects to the *CLC Server* it automatically detects if Secure Socket Layer (SSL) should be used on the port it is connecting to or not.

If SSL is detected, the server's certificate will be verified and a warning is displayed if the certificate is not signed by a recognized Certificate Authority (CA) as shown in figure 17.1.

When such an "unknown" certificate has been accepted once, the warning will not appear again. It is necessary to log in again once the certificate has been accepted.

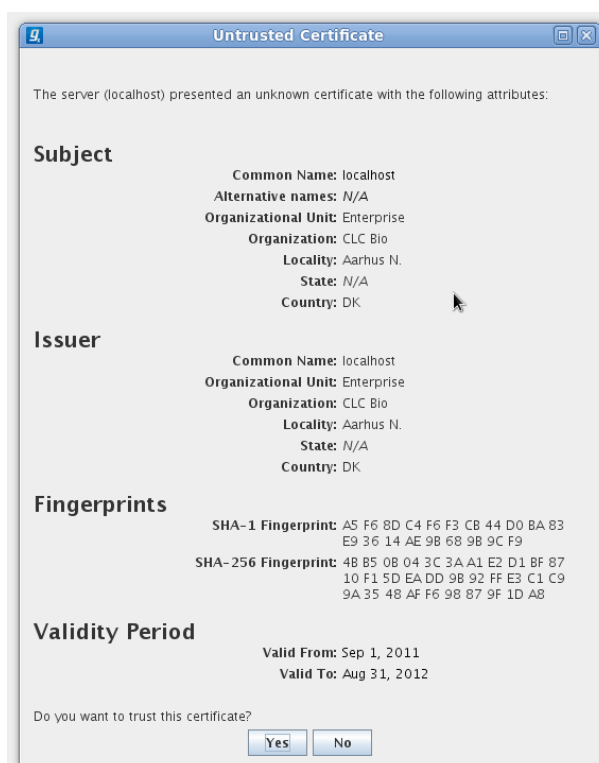


Figure 17.1: A warning is shown when the certificate is not signed by a recognized CA.

When logged into a server, information about the connection can be viewed by hovering the connection icon on the status-panel as shown in figure 17.2.

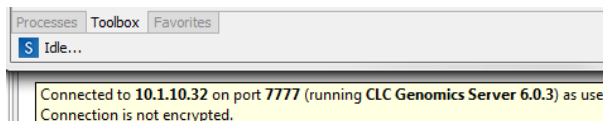


Figure 17.2: Showing details on the server connection by placing the mouse on the globe.

The icon is gray when the user is not logged in, and a pad lock is overlaid when the connection is encrypted via SSL.

17.3.3 Logging in using SSL from the CLC Server Command Line Tools

The CLC Server Command Line Tools will also automatically detect and use SSL if present on the port it connects to. If the certificate is untrusted the `clcserver` program will refuse to login:

```
./clcserver -S localhost -U root -W default -P 8443
Message: Trying to log into server
Error: SSL Handshake failed. Check certificate.
Option          Description
-----
-A <Command>    Command to run. If not specified the list of commands on the server will be returned.
-C <Integer>    Specify column width of help output.
-D <Boolean>    Enable debug mode (default: false)
-G <Grid Preset value> Specify to execute on grid.
-H             Display general help.
-I <Algorithm Command> Get information about an algorithm
-O <File>       Output file.
-P <Integer>    Server port number. (default: 7777)
-Q <Boolean>    Quiet mode. No progress output. (default: false)
-S <String>    Server hostname or IP-address of the CLC Server.
-U <String>    Valid username for logging on to the CLC Server
-V           Display version.
-W <String>    Clear text password or domain specific password token.
```

In order to trust the certificate the `clsserversslstore` tool must be used:

```
./clsserversslstore -S localhost -U root -W default -P 8443
The server (localhost) presented an untrusted certificate with the following attributes:
SUBJECT
=====
Common Name       : localhost
Alternative Names : N/A
Organizational Unit: Enterprise
Organization      : CLC Bio
Locality          : Aarhus N.
State             : N/A
Country           : DK

ISSUER
=====
Common Name       : localhost
Organizational Unit: Enterprise
Organization      : CLC Bio
Locality          : Aarhus N.
State             : N/A
Country           : DK

FINGERPRINTS
=====
SHA-1             : A5 F6 8D C4 F6 F3 CB 44 D0 BA 83 E9 36 14 AE 9B 68 9B 9C F9
SHA-256           : 4B B5 0B 04 3C 3A A1 E2 D1 BF 87 10 F1 5D EA DD 9B 92 FF E3 C1 C9 9A 35 48 AF F6 98 87 9F 1D A8

VALIDITY PERIOD
=====
Valid From        : Sep 1, 2011
Valid To          : Aug 31, 2012
Trust this certificate? [yn]
```

Once the certificate has been accepted, the `clserver` program is allowed to connect to the server.

17.4 Non-exclusive Algorithms

Below is a list of algorithms which are non-exclusive, meaning that multiple jobs of these types can be run concurrently on a given node, be that a single server, job or grid node.

Algorithms marked as *Streaming* are I/O intensive and two streaming algorithms will not be run at the same time. When running on grid, *Streaming* algorithms are treated as exclusive, meaning that they will never run in conjunction with other algorithms (or themselves).

Algorithm	Streaming
Add attB Sites	
Amino Acid Changes	X
Annotate and Merge Counts (legacy)	
Annotate from Known Variants	X
Annotate with Conservation Scores	X
Annotate with Exon Numbers	X
Annotate with Flanking Sequences	X
Annotate with Nearby Gene Information	
Annotate with Overlap Information	X
Assemble Sequences	
Assemble Sequences to Reference	
BLAST at NCBI	
ChIP-Seq Analysis	
ChIP-Seq Analysis (legacy)	
Compare Sample Variant Tracks (legacy)	X
Convert DNA To RNA	X
Convert from Tracks	X

Algorithm	Streaming
Convert RNA to DNA	X
Convert to Tracks	X
Count-based statistical analysis	
Whole Genome Coverage Analysis	
Create Alignment	
Create BLAST Database	
QC for Read Mapping	
Create Entry Clone (BP)	
Create Expression Clone (LR)	
Create GC Content Graph Track	
Create Histogram	
Create Mapping Graph Tracks	
QC for Targeted Sequencing	
Create Track List	
Create Tree	
Demultiplex Reads	
Download 3D Protein Structure Database	X
Empirical Analysis of DGE	
Extract and Count (legacy)	
Extract Annotations	
Extract Consensus Sequence	
Extract Reads	
Extract Sequences	X
Fasta High-Throughput Sequencing Import	X
Remove Variants Present in Control Reads	X
Filter against Known Variants	X
Filter Annotations on Name	X
Filter Based on Overlap	X
Remove Marginal Variants	X
Remove Reference Variants (legacy)	X
Find Binding Sites and Create Fragments	
Find Open Reading Frames	
Identify Enriched Variants in Case vs Control Samples	X
GO Enrichment Analysis	
Identify Graph Threshold Areas	
Illumina High-Throughput Sequencing Import	X
Import SAM/BAM Mapping Files	X
Import Tracks from File	
InDels and Structural Variants	
Ion Torrent High-Throughput Sequencing Import	X
Link Variants to 3D Protein Structure	X
Merge Annotation Tracks	X
Merge Overlapping Pairs	
Merge Read Mappings	X
Motif Search	
Gaussian Statistical Analysis	
Predict Splice Site Effect	

Algorithm	Streaming
Probabilistic Variant Detection	
Quality-based Variant Detection	
Reverse Complement Sequence	
Roche 454 High-Throughput Sequencing Import	X
Sanger High-Throughput Sequencing Import	X
Secondary Peak Calling	
Translate to Protein	
Trim Sequences	
TRIO analysis	

17.5 DRMAA libraries

Distributed Resource Management Application API (DRMAA) libraries are provided by third parties. Please refer to the distributions for instructions for compilation and installation, and contact the DRMAA providers if problems arise. QIAGEN Bioinformatics Support is not able to troubleshoot DRMAA library issues.

Information in this section of the manual is provided as a courtesy, but should not be considered a replacement for reading the documentation that accompanies the DRMAA distribution itself.

17.5.1 DRMAA for SLURM

Information about DRMAA for SLURM can be found at <https://slurm.schedmd.com/download.html>.

17.5.2 DRMAA for LSF

The source code for this library can be downloaded from <https://github.com/PlatformLSF/lsf-drmaa>. Please refer to the documentation that comes with the distribution for full instructions. Of particular note are the configure parameters "--with-lsf-inc" and "--with-lsf-lib" parameters, used to specify the path to LSF header files and libraries respectively.

17.5.3 DRMAA for PBS Pro

Source code for this library can be downloaded from <http://sourceforge.net/projects/pbspro-drmaa/>.

Please refer to the documentation that comes with the distribution for full instructions. Of particular note is the inclusion of the "--with-pbs=" parameter, used to specify the path to the PBS installation root. The configure script expects to be able to find lib/libpbs.a and include/pbs_ifl.h in the given root area, along with other files.

Please note that SSL is needed. The configure script expects that linking with "ssl" will work, thus libssl.so must be present in one of the system's library paths. On Red Hat and SUSE you will have to install openssl-devel packages to get that symlink (or create it yourself). The install procedure will install libdrmaa.so to the provided prefix (configure argument), which is the file the CLC Server needs to know about.

The PBS DRMAA library can be configured to work in various modes as described in the README file of the pbs-drmaa source code. We have experienced the best performance, when the CLC Server has access to the PBS log files and pbs-drmaa is configured with wait_thread 1.

17.5.4 DRMAA for OGE or SGE

OGE/SGE comes with a DRMAA library.

17.6 Consumable Resources

Setting up Consumable Resources with LSF

The following information was provided by IBM.

If you have questions or issues with setting up a consumable resource for LSF, please refer to your LSF documentation. For questions not covered there, please contact ruzhuchen@us.ibm.com and achristi@ca.ibm.com.

LSF has the ability to do "license scheduling" and ensure that CLC Server jobs running under LSF are only dispatched when there are available CLC Grid Worker licenses. When such scheduling is configured, CLC jobs for which no free licenses are available would stay in "pend" status, waiting for a CLC Grid Worker license to become available.

There are two parts to making use of this type of scheduling:

1. Configure the consumable resource in LSF.
2. Specify a clcbio license reservation when jobs are submitted to LSF.

Configuring the consumable resource in LSF

Add a consumable resource called clcbio in \$LSF_ENVDIR/lsf.shared:

```
Begin Resource
RESOURCENAME  TYPE  INTERVAL  INCREASING  DESCRIPTION # Keywords
    mips        Boolean  ()          ()           (MIPS architecture)
...
...
    clcbio      Numeric  ()          N            (clcbio license)
End Resource
```

Add the number of clcbio licenses in \$LSF_ENVDIR/lsf.cluster.<clustername>:

```
Begin ResourceMap
RESOURCENAME  LOCATION
# CLCBIO license resource
clcbio        (14@[all]) # 14 clcbio licenses can be used
#....
End ResourceMap
```

This example shows a configuration for 14 CLC Grid Worker licenses, which means that up to 14 CLC jobs can be running on the LSF cluster at the same time. This integer needs to be changed to the number of licenses you own.

The configuration shown here assumes the CLC Grid Worker licenses can only be use in the LSF cluster as LSF will manage the free token count from the scheduling side.

In this context, LSF does not replace or directly talk to the LMX license server for CLC licenses. Rather, LSF manages the CLC Grid Worker license reservations internally.

Specify a clcbio license reservation when jobs are submitted to LSF

CLC jobs submitted to LSF need to have a clcbio license reservation specified.

This can be done in several different ways:

- via the CLC Grid Preset "Native Specification" field. (This is the most convenient method.)
Simply add:

```
-R "rusage[clcbio=1]"
```

to this field.

- via the batch job submission command line
- using the RES_REQ line inside the lsb.queues file
- via an application profile (lsb.applications)

Important: After any LSF configuration file changes, one needs to reconfigure LSF for the changes to take effect. That is, run:

```
lsadmin reconfig  
badmin reconfig
```

These are "safe" commands to run. That is, pending LSF jobs will continue to "pend" in status and running LSF jobs will continue to run.

17.7 Third party libraries

The *CLC Server* includes a number of third party libraries.

Please consult the files named NOTICE and LICENSE in the server installation directory for the legal notices and acknowledgements of use.

For the code found in this product that is subject to the Lesser General Public License (LGPL) you can receive a copy of the corresponding source code by sending a request to our support team at ts-bioinformatics@qiagen.com.

17.8 External network connections

Some functionality available in CLC software requires access to specific addresses on the Internet. A list of the internet sites accessed and a listing of the tools involved can be found at <https://qiagen.secure.force.com/KnowledgeBase/KnowledgeNavigatorPage?id=kA41i00000L5smC>

The list of sites there can be referred to when configuring firewall settings for networks that utilize a whitelist approach. For CLC Servers with nodes, any nodes that need to execute functionality listed on that webpage will need access to the relevant sites.

17.8.1 Proxy settings

To add proxy settings to the CLC server, you will need to add lines to the server `.vmoptions` file. This file can be found in the installation area of the CLC server software. The name will reflect the specific product. For example, for the CLC Genomics Server, it would be called `CLCGenomicsServer.vmoptions`.

The following lines must be added to that file:

```
-Dhttp.proxyHost=  
-Dhttp.proxyPort=  
-Dhttp.nonProxyHosts="localhost|127.0.0.1|11...|.foo.com|etc"
```

where the `proxyHost` IP address and the `proxyPort` port number need to be added to complete the top two lines.

For job nodes, the settings described here must be applied to each node that will need to submit jobs that need access to the internet. For the `nonProxyHosts` values in this case, specify the names or IP addresses/subnets for *all* job nodes (if applicable with your server configuration) that should not be using the proxy service, if relevant.

For grid node setups, a `clcgridworker.vmoptions` file must be created in each deployed gridworker area, if such a file does not already exist and the settings described above added. See also section [6.3.10](#).

17.9 Read Mapper Reference Caching

In some cases, repeated mappings against the same reference will result in a dramatically reduced runtime because the internal data structure used for mapping the reads, which is reference specific, can be reused. This has been enabled by storing files in the system tmp folder as a caching mechanism. Only a certain amount of disk space will be used and once reaching the limit, the oldest files are cleaned up. Consequently, the reference data structure files will automatically have to be recreated if the cache was filled or the tmp folder was cleaned up.

The default space limit is 16 GB.

The reference cache size can be changed by creating a file called `readmapper.properties`, with an entry `referencecachesize = <size in bytes>`, for example
`referencecachesize = 8589934592`

A copy of this file should then be placed into the `settings` folder in the following locations:

- Under the installation area of the *CLC Server* on the single server or master node.
- Under the installation area of the *CLC Server* of each job node in a job node setup.
- Under each grid worker folder defined in your grid presets on a grid node setup.

17.10 Monitoring

We recommend that you monitor the health and performance of the servers that the *CLC Server* software is running on and also monitor some key metrics of the *CLC Server* itself. This will enable you to react quickly to any problems that occur and can aid in optimization of server performance.

With regards to the servers' physical resources, monitoring the amount of free memory and disk space is recommended, as consumption of these can be substantial depending on types and numbers of analyses being run.

Monitoring metrics of the *CLC Server* itself enables you to keep tabs on how well the jobs processing is going. The metrics the *CLC Server* provides are available as JMX¹ attributes. Software from a third party will be necessary to set up the monitoring of these attributes. Numerous software products for this are available and most support JMX. If your monitoring software supports the raising of alarms, you can set up triggers based on these metrics to receive alerts when a situation arises that needs attention.

17.10.1 Setting up JMX monitoring

No special configuration is necessary if monitoring will take place locally. However, JMX must be enabled for remote monitoring. This is done by adding a few settings to the server `vmoptions` file. The relevant `.vmoptions` file is located in the root of the server installation folder of a single server, or the root of the installation folder of the master server in the case of a node setup (Hereafter this folder will be referred to as `CLC_SERVER_BASE`).

Enable JMX with no security Add the following to the `.vmoptions` file:

```
-Dcom.sun.management.jmxremote.port=9999
-Dcom.sun.management.jmxremote.ssl=false
-Dcom.sun.management.jmxremote.authenticate=false
```

Enable JMX with authentication

1. Add the following to the `.vmoptions` file, instead of the lines provided in the section above.

```
-Dcom.sun.management.jmxremote.port=9999
-Dcom.sun.management.jmxremote.ssl=true
-Dcom.sun.management.jmxremote.authenticate=true
-Dcom.sun.management.jmxremote.password.file=../conf/jmxremote.password
-Dcom.sun.management.jmxremote.access.file=../conf/jmxremote.access
```

¹https://en.wikipedia.org/wiki/Java_Management_Extensions

2. Create the access authorization file `CLC_SERVER_BASE/conf/jmxremote.access` and write the following in it:

```
monitorRole readonly
controlRole readwrite
```

3. Create the password file `CLC_SERVER_BASE/conf/jmxremote.password` and write the following in it:

```
monitorRole clcserver
controlRole clcserver
```

Further information about setting up JMX monitoring can be found in the Oracle guide on Monitoring and Management Using JMX Technology <http://docs.oracle.com/javase/8/docs/technotes/guides/management/agent.html>.

17.10.2 Completed process metrics

Object name: `com.clcbio.server:type=CompletedProcesses`

The "completed process" metrics can be used to evaluate the processes that are complete either because they were successful or because they failed. Canceled processes are ignored. The *CLC server* provides a temporal view of the latest completed processes, with two different temporal views available: time frame view or a history view that includes a fixed number of the most recently completed processes.

The size of the time frame to view and the number of entries for the history view can be configured directly through JMX or by editing the `Monitoring.properties` file. This properties file is located in this folder: `CLC_SERVER_BASE/settings/`. Please change the default settings to values that fit your specific setup. Lower values will generally result in a more reactive monitoring solution, but values that are too low may result lead to false alarms.

The following is a list of all the process related metrics that are available:

Number of processes in history

Attribute name: `NumberOfProcessesInHistory`

The number of processes currently in the history. Successful and failed processes are included. Canceled processes are not included. The maximum size of the history can be set using the `SizeOfHistory` attribute, available through JMX and the configuration file.

Number of failed processes in history

Attribute name: `NumberOfFailedProcessesInHistory`

The number of failed processes currently in the history.

Fraction of failed processes in history

Attribute name: `FractionOfFailedProcessesInHistory`

The fraction of the processes in the history that have failed. This fraction is not of much value if the number of processes in the history is very low.

Number of processes within time frame

Attribute name: `NumberOfProcessesWithinTimeFrame`

The number of processes that have been completed between now and a variable number of milliseconds earlier. Both successful and failed processes are included. Canceled processes are not included. The time frame can be set using the `TimeFrameInMilliseconds` attribute, that is available through JMX and the configuration file.

Number of failed processes within time frame

Attribute name: `NumberOfFailedProcessesWithinTimeFrame`

The number of failed processes that have been completed between now and a variable number of milliseconds earlier.

Fraction of failed processes within time frame

Attribute name: `FractionOfFailedProcessesWithinTimeFrame`

The fraction of failed processes compared to the total number of processes that have been completed between now and a variable number of milliseconds from now. This fraction is not of much value if the number of processes in the time frame is very low.

17.10.3 Process execution metrics

Object name: `com.clcbio.server:type=ProcessExecution`

Process execution metrics allow measurement of how many jobs are being processed and how many are in a queue because they are waiting for available processing resources.

On job node setups, the object names are available on all nodes, but it only makes sense to monitor them on the master node since this is where the jobs are managed. If a grid is used to process the jobs, the actual queue will be a part of the grid system, which results in the processes being moved almost instantly to the "currently processing" state and the *CLC Server* queue itself is then empty.

Currently processing

Attribute name: `CurrentlyProcessing`

Number of processes being executed at the moment.

Waiting for resources

Attribute name: `WaitingForResources`

On a job node setup, the number of processes that are queued and are waiting for a node to be available for processing. This does not include processes that are waiting for output from another process. It includes only processes that have the input they need and are ready to be processed, but where no resources are available at that moment.

17.10.4 Job node metrics

Object name: `com.clcbio.server:type=JobNodes`
`com.clcbio.server:type=JobNodes,name=<job node name>`

With the job node metrics you can monitor a master node's connection with its job nodes. The object name is available on all nodes, but it only makes sense to monitor this on the master node. There are two sets of attributes to monitor. One set provides an aggregated view of all the job nodes while the other provides individual attributes for each job node.

Communication errors are only reported if the server uses the General queue. If the High throughput queue is used, the master node never contacts the job nodes on its own initiative and therefore there is no support for monitoring the job nodes through JMX in the current version of the server.

Apart from communication error attributes, the set of individual attributes also includes information about the host and port of a given job node. This information is not meant for monitoring as such, but is included for convenience, as when an error does arise identification of the job node involved is usually necessary.

Communication failed

Attribute name: `CommunicationFailed`

This attribute is set to true if the master node is currently having problems communicating with this particular job node.

Seconds since communication failed

Attribute name: `SecondsSinceCommunicationFailed`

The number of seconds since the communication with the job node first failed. As soon as the master node succeeds in connecting with the job node again, this value returns to zero. This attribute can be useful if you want to avoid reacting to very short fallouts in communication.

Max seconds since communication failed

Attribute name: `MaxSecondsSinceCommunicationFailed`

The maximum number of seconds since communication with any of the job nodes first failed. The advantage of this metric is that monitoring of it can be set up once and does not need to be changed if a job node is attached or detached.

Number of job nodes

Attribute name: `NumberOfJobNodes`

The number of job nodes currently attached to the master server.

Number of failed job nodes

Attribute name: `NumberOfFailedJobNodes`

The number of job nodes the master server currently has problems communicating with.

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