

INTRODUCTION

LINK is a software solution for automated acquisition, processing, and reporting of data produced by analytical instruments. LINK will search network locations for new data files that have been produced by analytical instrument software, extract all useful information from these data files (instrument settings, parameter calculations, fully xy curve datasets), and copy this data to a centralized database. A powerful analysis user interface allows datasets to be aggregated, overlaid, grouped based on metadata, and visualized in the form of charts/tables/images from which Word and PDF reports may be generated.

In addition to fully automated custom Word/PDF report generation, LINK provides a convenient and secure repository for both project data and corresponding analysis/visualization templates. The software is available in a 21CFR Part11 compliant format, should cGMP application be required. For advanced interaction with other data management systems, LINK is equipped with a fully featured API for programmatic data acquisition/processing/retrieval. LINK also supports export to other database systems.

LINK SOFTWARE COMPONENTS

LINK utilizes a client/server-based architecture. The LINK server software is installed on computing hardware provided by the end-user (on-premises solution). It consists of a MySQL (MariaDB) database, Apache Tomcat webserver, and Java-based data processing engine. The LINK installation bundle includes all required third party software (MariaDB, Apache Tomcat, and Java), and is fully supported by Lumetics.

The LINK Client is a dedicated browser-based application built on the Chromium platform. It is fully portable, consisting of a folder with supporting files plus the link.exe application. The LINK client is placed on the LINK Server computer and all office/lab PCs that users may wish to use to connect to the LINK server. For added convenience the LINK client may also be launched directly through the Chrome or Edge browser.

Client/server communication occurs over http port 8080 by default, however, an alternative port number may be selected and applied at the point of installation should this be requested. Client/server communication may be configured to utilize https for secure communication, and LDAPS for secure authentication. If this is of interest, please contact your Lumetics representative for further discussion regarding configuration and installation of security certificates.

LICENSES, USERS, & LOGIN

User Licenses: Annual user license subscriptions are required to login to LINK. LINK user license subscriptions are concurrent. E.g., if four license subscriptions are purchased, any four users may login simultaneously to import/analyze/export data. LINK may be configured to support an unlimited number of read-only viewer logins, where LINK-processed data may be viewed but not modified.

Server Licenses: Annual license subscriptions are required to enable advanced or specialized LINK server capabilities. Examples of LINK server licenses include API, Machine Learning, and Database Export. Other examples include LINK server/database nodes if clustering is utilized.

User Privileges: Five types of users may be specified: Administrators, Super Users, Analysts, Reviewers, and Read-only Viewers. Typically, Windows user groups are set up for each user level, and users are assigned membership into one or more of these groups. However specific users and their associated privilege may also be 'hard-coded' into the LINK license file. The privileges afforded each group are fully configurable within the LINK software itself.

User Login: LINK may be configured to support Windows login credentials, and use of LDAPs if required.



LINK NETWORK DIAGRAM



The LINK software platform fully automates the process of locating data files on the network, parsing all useful information, copying that data to a centralized database, adding metadata, analyzing results, and producing reports. The LINK automated solution provides read access to both source and LINK-processed data through the LINK client interface, as well as a wide range of export options permitting seamless data transfer to many other data management systems.

In addition to an automated routine analysis and advanced data interrogation, LINK supports file capture (source and ancillary) to view and download as required. Additionally, the LINK solution is 21 CFR Part 11 compliant and has been successfully validated for cGMP.

LINK is a web-based client-server architecture, communicating via http (or https). It is an 'on-premise' solution where data storage and access remains fully under the user's company IT control.

Lumetics provides the required server software: MariaDB MySQL database, Apache Software Foundation Tomcat 9 webserver, and Java. The Tomcat 9 webserver runs under Windows account credentials that enable searching Windows file share locations for source data (read access privileges required), and report writing to Windows file share locations (write access privileges required).

The desktop LINK client is a portable stand-alone web application (admin rights not required for installation). Chrome or Edge may also be utilized for LINK server connection (with minimal feature exclusions). User login and authentication apply Windows AD and Idap (or Idaps) where users are assigned to one of five configurable user levels (Administrator, Super User, Analyst, Reviewer, or Read Only Viewer).

* For optimal performance, the LINK server + database(s) and any Machine Learning servers should be in close network proximity to the source data. Use of multiple separate LINK servers at different sites or cloud file share network locations may be advisable. LINK clients may conveniently connect to any LINK server for which they have access permission.

RECOMMENDED LINK SERVER HARDWARE SPECIFICATIONS

The table below is a useful starting point for assigning appropriate computing resources to the LINK server and database. LINK performance is highly dependent on the number of concurrent users, available CPUs, hard drive read/write speeds, network conditions, and LINK usage patterns. Lumetics recommends running its benchmark performance data sets for performance optimization!

Attribute	1-5 licenses	5-10 licenses	10-15 licenses	15-20 licenses
Effective CPUs (Cores X Threads/Core)	12	16	20	24
RAM	16 GB	16 GB	16 GB	24 GB
Hard Drive Free Space	≥ 100 GB			
Operating System	Minimum: Windows 7+ or Win Server 2008+, 64-bit OS			
CPU Clock Speed	≥ 4 GHz			
Disk R/W Speed	≥ 3000 MB/s (typically SSD)			
Storage Configuration	Separate drives for System OS and Database			
Network Speed	≥ 1 Gbps (between data source and LINK Server)			
** For licenses >=20, please contact Lumetics to discuss Server Configuration options.				



LINK INSTALLATION AND CONFIGURATION OPTIONS

At a minimum, a computer must be designated to be the LINK server where both the server and database shall reside. Both the LINK server and desktop client shall be installed on this computer. Following this, users may login at the LINK server computer itself and import data that is stored locally. This can be helpful for software evaluation or when only a single user is utilizing the software. The following configuration options provide higher levels of user convenience, data security, and utilization scalability. These options do not need to be applied at the point of installation and may be applied as/when required.

Basic Installation Options

- A. Networked Data Import: this option permits searching the network for instrument data files, in addition to them being located on the LINK server computer itself. The LINK server (via Apache Tomcat) must run under a set of Windows login credentials that possess read access to the network locations where data files reside. A Windows Service Account is typically set up for this purpose, to help ensure continuous service availability.
- B. Remote Client Access: this option permits connecting to the LINK server and logging in from the desktop LINK Client that has been placed on user PCs (or via Chrome/Edge browser) and requires network connectivity to the LINK server computer.
- C. Windows Login: this option permits users to login using their Windows login credentials, instead of usernames that have been hard coded into the Lumetics license file. To enable this feature, Lumetics requires the address of the LDAP server (e.g., "ldap://dom065.amer.lumetics.com:389"), the CN or OU for users (e.g., USERS, or ACCOUNTS/USA), and the Windows usernames of each LINK user and their associated privileges (Administrator, Super User, Analyst, Reviewer, or Read Only Viewer). Or, in place of the Windows names of each LINK user, the names of the Windows User Groups created for the user levels.

Advanced/Specialized Options

- A. Electronic Signatures: this option is typically selected for cGMP application and triggers a requirement for users to enter their password upon each LINK transaction that affects data and/or data visualization. This feature can only be enabled by your Lumetics installation technician.
- B. Reviewer Signoff: if Electronic Signatures have been enabled, there is an option for Reviewer signoff upon PDF report generation. Reviewer Signoff requires a Windows User Group of Reviewers to be in place, that defines those users who may also act as authorized Reviewers.
- C. LDAPs/https: This option is usually selected if secure LDAPs or https transactions are required. Please contact Lumetics to arrange the creation and placement of the required security certificates.
- D. LINK MariaDB MySQL Database on a separate LINK server computer drive, or separate computing system
- E. Clustered database systems and/or multiple LINK Data Management Systems such that LINK server and database(s) remain in close network proximity to source data files for optimal performance.
- F. LINK Machine Learning: This option is usually selected if an end user wishes to connect to a TensorFlow Serving system to apply machine learning models to LINK images/data. It requires that the Machine Learning capability be enabled in your LINK server license file (i.e., a ML subscription has been purchased for the LINK server).
- G. LINK API: This option is usually selected if an end user wishes to access raw or LINK-processed data programmatically or trigger a report generation via URL requests of the LINK server. It requires that the API capability be enabled in your LINK server license file (i.e., a LINK API subscription has been purchased for the LINK server).
- H. LINK Database Export: This option enables export of LINK processed data to an external database, that may be queried directly by other systems such as ELNs, Spotfire, Tableau etc..... It requires that the Database Export capability be enabled in your LINK server license file (i.e., a Database Export subscription has been purchased for the LINK server).

*** Please contact your Lumetics Representative for download links, license files, and installation instructions that are specific to your LINK purchase agreement.



LINK SERVER AND CLIENT INSTALLATION

LINK Installation Process:

- 1. Download and run the LINK component installer (installs Java, MariaDB, and Tomcat): cplease obtain download link from Lumetics>
- 2. Download and run the latest LINK server update: cplease obtain download link from Lumetics>
- Download and run the latest LINK desktop client. This will place a copy of the client folder in C:\Lumetics LINK Client (64-bit), and a copy of the link.exe on the desktop:
 <please obtain download link from Lumetics>
 This is preferred over Chrome/Edge client connection due to more features being available.
- 4. Place the link.lic license file provided by Lumetics here on the LINK server computer: C:\Program Files\Apache Software Foundation\Tomcat 9.0\webapps\lumeticslink
- 5. Open the Services tab, right click on the Tomcat/Apache Tomcat service, select Properties, select the Log On tab, and enter the Windows credentials that your LINK server is to run under. This account will determine which locations/folders on the network the LINK server has read access to. If an account is not provided, data may only be imported that is local to the LINK server computer.
- 6. Right click on each of the Program Files\Apache Software Foundation folder and ProgramData\LumeticsLINK folder, select Properties, select the Security tab, and ensure that the windows account used for Tomcat is present and has Full Control (selecting the Advanced button, you can add new users as required).

Installation Verification Process:

- Download sample MFI data: https://lumetics.box.com/s/io8jcyrixw04928a1h2mhmm2ct78qa5r
- Data import and manipulation verification:
 - Launch the LINK client (run the link.exe or connect via Chrome).
 - \circ ~ Login using windows credentials or with the username provided by Lumetics.
 - Place the sample MFI data on the server desktop or C:, and verify the ability to import MFI 4200/5200 data to a LINK project
 - Place the sample MFI data on the network where end user data shall reside and verify the ability to import MFI 4200/5200 data to a LINK project from that network location.
 - Launch an analysis of a project, drag down any dashboard, and verify the ability to view thumbnail images and generate a Word report.
- Verify LINK desktop client connectivity by running the LINK desktop client updater on any end-user PC, running the link.exe, and in the top right corner left click "Server:localhost" and replacing "localhost" with the name of the LINK server. Verify the ability to successfully connect and login.
- Verify LINK browser client connectivity by launching Chrome/Edge, entering
 "ServerName:8080/lumeticslink/login.html" into the browser address bar (replacing "ServerName" with the name of
 the LINK server), and verifying the ability to successfully login.
- Please contact Lumetics for direct assistance, a review of additional configuration/security/installation options, and training using the LINK software!



TENSORFLOW SERVING INSTALLATION (OPTIONAL)

TensorFlow Serving Installation:

For application of Machine Learning within LINK, a TensorFlow Serving instance that is serving one or more models must be configured and accessible to the LINK server over port 8501. The TensorFlow Serving computer should meet the following specifications:

- RAM: 16 Gb or higher
- CPU: 8 core or higher (faster/newer the better)
- GPU: optional compatible NVIDIA GPU is not required, but will help with image processing speed
- OS: Ubuntu 20.04
- Other 3rd Party Software: Docker, latest available version
- Network: high speed proximity/connectivity to the LINK server (this can be highly influential on data import speeds when larger numbers of images are involved)

Configuration of the TensorFlow Serving computer consists of the following steps:

- 1. Install NVIDIA driver (if applicable): https://docs.nvidia.com/datacenter/tesla/tesla-installationnotes/index.html#ubuntu-lts
 - o SKIP the "post installation steps" instructions, as these are not needed
- 2. Install Docker: https://docs.docker.com/engine/install/
 - Choose Linux distro in the below link, and follow the steps to install "Using the Repository", and select "install the latest version" wherever applicable (they sometimes have steps to install a specific version of Docker, which we do not want to do)
- 3. Install NVIDIA toolkit: https://docs.nvidia.com/datacenter/cloud-native/container-toolkit/install-guide.html#docker
 - Find the section representing your Linux Distro.
 - SKIP the first section "Setting up Docker" which installs Docker (we did this above using the official site instructions for that)
 - Scroll down to the section in your Linux distro that says, "Setting up NVIDIA Container Toolkit" and start from that point onwards. Follow their test example to verify the driver is installed.
- 4. Test Docker with GPU by running this:
 - o Run this command: sudo docker run --gpus all --rm nvidia/cuda nvidia-smi
 - Should output some info about the GPU to indicate success. A failure will be a crash of the container.
- 5. Install TensorFlow/serving docker containers
 - With GPU support
 - Run this command: sudo docker pull tensorflow/tensorflow:latest-gpu
 - Run this command: sudo docker pull tensorflow/serving:latest-gpu
 - Without GPU Support
 - sudo docker pull tensorflow/serving
 - sudo docker pull tensorflow/tensorflow
- 6. Serve machine learning models (please consult Lumetics for specific instructions)
 - Apply the Lumetics python script to your saved model, readying it for serving
 - o Establish a tensorflow serving Docker container
 - Serve the model within the Docking container
 - Create a TensorFlow connection in the LINK server and test for connectivity
 - Utilize one or more models in LINK Import Methods

CONTACT LUMETICS

For direct assistance, please contact Lumetics LINK[™] Support: E-mail: support@lumetics.com Phone: 1.613.417.1839 Website: http://lumetics.com/

