

MPI Topological Material Database Web-Application

Installation on a Linux Server

Abstract

<todo>

Description

The Application consists of two parts

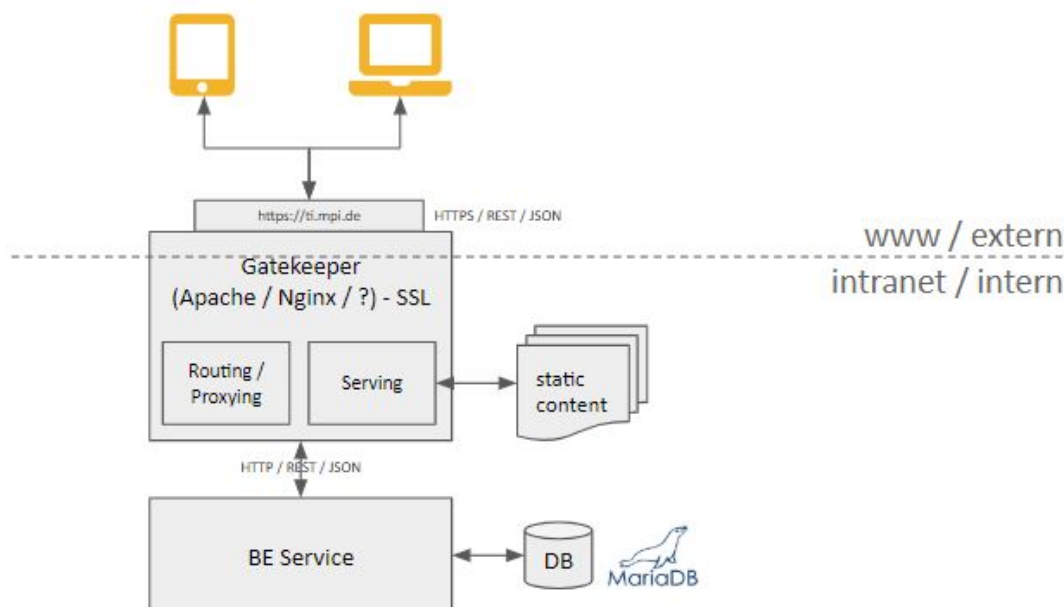
1. the Backend Part, which is a self running Java Package, which is responsible for

- Rest API
- Data (Pre-) Processing
- Parsing
- Access to the Database

2. the Frontend Part, which is a vue.js based Application, which is responsible for

- accessing the Backend Rest API
- Client Behaviour on all kind of devices
- Visualization

The Architecture



Prerequisites

The Backend Server used Java 8+, recommended JDKs are: Oracle JDK or OpenJDK

The Application was build using: **java version "1.8.0_191"**

Java Installation Successful, if
<pre># java -version java version "1.8.0_191" Java(TM) SE Runtime Environment (build 1.8.0_191-b12) Java HotSpot(TM) 64-Bit Server VM (build 25.191-b12, mixed mode)</pre>

1. A domain, lets assume topologicalmaterials.com, is needed
2. A sub-domain for the Backend-Service Proxy is needed, such as api.topologicalmaterials.com; alternatively a resource, such as: topologicalmaterials.com/api/
3. A sub-domain for the nonallycompound files is needed, such as files.topologicalmaterials.com, is needed; alternatively a resource, such as: topologicalmaterials.com/files/
4. A sub-domain for the web/www files is needed, such as www.topologicalmaterials.com, is needed; alternatively a resource, such as: topologicalmaterials.com/www/
5. A sub-domain for the Seekpath is needed, such as seekpath.topologicalmaterials.com, is needed; alternatively a resource, such as: topologicalmaterials.com/seekpath/
6. SSL Certificate(s) for this domain(s)

The Installation

The *Backend* part is a standalone application, which is configured via so called JVM Parameters. The Service itself, works on a model, which is called **Immutable Server**. Means: there is no configuration change, after a server has started. The configuration is bundled and fixed within startup. See here: <https://martinfowler.com/bliki/ImmutableServer.html>

The Application is built in a way, that it ONLY binds to "localhost/127.0.0.1", it is not accessible from the outside, as it is hidden behind a Gatekeeper. If this needs to be changed, change the Variable SERVER_ADDRESS to remove this limitation.

The Server manages the database migrations and Schema validation is done using Hibernate. Once the database changes existing / used Tables / Columns, the Server will not startup, if the types are not compatible.

The *Frontend* part is a bundled web-application containing HTML, CSS, JS, ... Files.

The *Released* package contains two Folders.

1. Backend: contains the jar File / the executable; such as mpi-backend-service-<version>.jar, e.g. mpi-backend-service-0.2.1.jar
2. Frontend: contains the web-application

Backend Installation: The Backend Parts needs to be executable / accessible by Java. A typical location is /var/opt/. The Server can be started using the following script / command.

It is recommended to configure this application as a service using e.g. systemd.

Startup Script / Startup Parameters

```
java -DSCHEDULER_ENABLED=true \  
-DSERVER_PORT=8080 \  
-DSTATIC_RESOURCE_NONALLOYCOMPOUNDS="http://mpi-static.domain.de/%s/%s" \  
-DDATASET_FOLDER="/var/www/html/mpi-static.domain.de/" \  
-DDB_URL="jdbc:mysql://localhost:3306/mpi_v7?serverTimezone=UTC&useSSL=false" \  
-DDB_USER_NAME=mpi_v7 \  
-DDB_PASSWORD=sommer \  
-DDB_SCHEMA=mpi_v7 \  
-jar mpi-backend-service-0.2.1.jar
```

Variable	Meaning	Allowed Value(s) / Unit
SCHEDULER_ENABLED	Global Setting to enable / disable Scheduling	true - enabled (default) false - disabled
SCHEDULER_CONTENT_PARSING	Scheduled check for outdated file information, which need to be updated / parsed	10000 msec (default)
SCHEDULER_CIF_PROCESSING	Scheduled check for outdated CIF File information, which need to be updated / parsed (and asked against	10000 msec (default)

	the CIF Webserver)	
SCHEDULER_SEARCH_REFRESH	Scheduled Check for outdated Search Index entries; given Compounds are added	30000 msec (default)
SERVER_ADDRESS	The Binding IP Address, it is recommended to not overwrite this setting.	127.0.0.1 (default)
SERVER_PORT	The listening Server Port	8080 (default)
STATIC_RESOURCE_NONALLOYCOMPOUNDS (mandatory)	Path where the Non-Alloy Compound Files can be found; This is a pattern http(s)://server/<datapath>/<file> whereas datapath relates to compounds.datapath and file relates files within this datapath, such as: compounds.cif, compounds.bspicfile, compounds.dospicfile, ...	http://mpi-static.domain.de/%s/%s
DATASET_FOLDER (mandatory)	Folder, where the scheduler can access "local" Data Files for parsing In this example, as the Files are served also through the Webserver, the www path is referenced (there is no relation of serving them via HTTP)	/var/www/html/mpi-static.domain.de/
DB_URL (mandatory)	JDBC Connection URL MySQL: jdbc:mysql://<server>:<port>/<dbname>?serverTimezone=UTC&useSSL=false MariaDB: jdbc:mariadb://<server>:<port>/<dbname>	MySQL: jdbc:mysql://localhost:3306/mpi_v7?serverTimezone=UTC&useSSL=false MariaDB: jdbc:mariadb://localhost:3307/mpi_v7
DB_USER_NAME (mandatory)	The name of the Database User	e.g. mpi_v7
DB_PASSWORD (mandatory)	The password of the Database User	e.g. mypassword
DB_SCHEMA (mandatory)	The (dedicated) Schema	e.g. mpi_v7
RESOURCE_CIF_SERVER (mandatory)	The HTTP resource of the CIF processing Webserver (see also Section CIF Server). The "process_structure" Resource is needed within this configuration.	http://mpi-seekpath.domain.de/process_structure/
HIDE_TI_EQUALS_ZERO	In Search Results hide TI with value 0	true - enabled (default) false - disabled
LEFTMOST_IDENTIFIER_GAPHIGHSYMPOINT	Rotation of the Gap High Sympoint Header having the specified value most left	default: Γ

LEFTMOST_IDENTIFIER_BANDREPRESENTATION	Rotation of the Band Representation Header having the specified value most left	default: GM
LEFTMOST_IDENTIFIER_SUBGROUPSTABLESUB	Rotation of the Subgroups Table Sub Entry Header having the specified value most left	default: GM
RATE_LIMIT_ENABLED		default:true
RATE_LIMIT_HOURLY		default:200
RATE_LIMIT_BAN_HOURS		default:12

Apache Configuration

The Apache runtime needs to serve three needs:

1. Providing the HTML, CSS, JS, ... to the clients
2. Providing the content from the nonalloycompounds folder to the clients
3. Proxy for the HTTP(s) calls to the Backend Service
4. Proxy for the HTTP(s) calls to Seekpath

The following configuration shows the configuration following the sub-domains approach.

The Apache needs to have the following modules enabled

```
sudo a2enmod proxy
sudo a2enmod proxy_http
```

1. Providing the HTML, CSS, JS, ... to the clients

Apache Configuration (SSL)
/etc/apache2/sites-available/topologicalmaterials.com.conf

```
<VirtualHost *:443>

    ServerAdmin webmaster@localhost
    ServerName mpi-static.topologicalmaterials.com
    DocumentRoot /var/www/html/www.topologicalmaterials.com/

    ErrorLog ${APACHE_LOG_DIR}/error.log
    CustomLog ${APACHE_LOG_DIR}/access.log combined

    Include /etc/letsencrypt/options-ssl-apache.conf
    SSLCertificateFile
    /etc/letsencrypt/live/www.topologicalmaterials.com/fullchain.pem
    SSLCertificateKeyFile
    /etc/letsencrypt/live/www.topologicalmaterials.com/privkey.pem

</VirtualHost>
```

Apache Configuration (Non-SSL)
/etc/apache2/sites-available/topologicalmaterials.com.conf

```
<VirtualHost *:80>

    ServerAdmin webmaster@localhost
    ServerName mpi-static.topologicalmaterials.com
    DocumentRoot /var/www/html/mpi-static.topologicalmaterials.com/

    ErrorLog ${APACHE_LOG_DIR}/error.log
    CustomLog ${APACHE_LOG_DIR}/access.log combined

</VirtualHost>
```

2. Providing the content from the nonalloycompounds folder to the clients

Apache Configuration (SSL)

/etc/apache2/sites-available/topologicalmaterials.com.conf

```
<VirtualHost *:443>

    ServerAdmin webmaster@localhost
    ServerName mpi-static.topologicalmaterials.com
    DocumentRoot /var/www/html/mpi-static.topologicalmaterials.com/

    ErrorLog ${APACHE_LOG_DIR}/error.log
    CustomLog ${APACHE_LOG_DIR}/access.log combined

    Include /etc/letsencrypt/options-ssl-apache.conf
    SSLCertificateFile
    /etc/letsencrypt/live/mpi-static.topologicalmaterials.com/fullchain.pem
    SSLCertificateKeyFile
    /etc/letsencrypt/live/mpi-static.topologicalmaterials.com/privkey.pem

</VirtualHost>
```

Apache Configuration (Non-SSL)

/etc/apache2/sites-available/topologicalmaterials.com.conf

```
<VirtualHost *:80>

    ServerAdmin webmaster@localhost
    ServerName mpi-static.topologicalmaterials.com
    DocumentRoot /var/www/html/mpi-static.topologicalmaterials.com/

    ErrorLog ${APACHE_LOG_DIR}/error.log
    CustomLog ${APACHE_LOG_DIR}/access.log combined

</VirtualHost>
```

3. the Proxy (SSL + Non-SSL), the 8080 points to the configured port in “-DSERVER_PORT=8080”

Apache Configuration

/etc/apache2/sites-available/topologicalmaterials.com-le-ssl.conf

```
<VirtualHost *:443>
    ProxyPreserveHost On
    ProxyPass "/" "http://localhost:8080/"
    ProxyPassReverse "/" "http://localhost:8080/"
    ServerName api.topologicalmaterials.com

    Include /etc/letsencrypt/options-ssl-apache.conf
    SSLCertificateFile
    /etc/letsencrypt/live/api.topologicalmaterials.com/fullchain.pem
    SSLCertificateKeyFile
    /etc/letsencrypt/live/api.topologicalmaterials.com/privkey.pem
</VirtualHost>
```

Apache Configuration (Non-SSL) /etc/apache2/sites-available/topologicalmaterials.com.conf
--

<VirtualHost *:80> ProxyPreserveHost On ProxyPass "/" "http://localhost:8080/" ProxyPassReverse "/" "http://localhost:8080/" ServerName mpi.leancoders.de </VirtualHost>

4. Proxy for the HTTP(s) calls to Seekpath, the configured Port, is the same port as exposed in the Docker Config **-p 8082:80 (expose internal Docker port 80 → local 8082)**, see also: Section CIF Server / Seekpath

We DO NOT need SSL here, as this application is “internally” used; HTTPS Handshake makes life harder.

Apache Configuration (Non-SSL) /etc/apache2/sites-available/topologicalmaterials.com.conf
--

<VirtualHost *:80> ProxyPreserveHost On ProxyPass "/" "http://localhost:8082/" ProxyPassReverse "/" "http://localhost:8082/" ServerName mpi-seekpath.leancoders.de </VirtualHost>
--

CIF Server / Seekpath

The Software uses an open source solution named seekpath, to generate a dataset, which is used to render the Brillouin Zone on the details page. The Software and installation instructions can be found here: <https://github.com/giovannipizzi/seekpath>

Note: During Development, it was unable to get Seekpath up and running with the WSGI bridge, therefore: It is recommended (as we have a running version) to use the provided Docker Environment / Container. The running version is using: Docker version 18.09.0, build 4d60db4
The environment can be spawned up using:

Docker Run Script / Command

<code>docker run -d --restart=always -p 8082:80 giovannipizzi/seekpath:latest</code>
--