

Updating an Existing MedeA Installation

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1 Introduction

This section describes the procedure to update your existing *MedeA* installation to *MedeA* 3.8. If you are installing *MedeA* for the first time, please refer to the Sections [Installing MedeA on Windows with the Windows Installer](#) and [Installing MedeA on Windows and Linux from ISO](#).

If you are updating to 3.8 from *MedeA* 3.1.0 and newer, you can use the Windows Installer or the ISO images available for download from <http://my.materialsdesign.com/download-medea-3.8>. You can also use the **Update from the Web** feature from the *MedeA Maintenance* program.

If you are updating to 3.8 from *MedeA* 3.0.X and older, please only use the ISO images available for download from <http://my.materialsdesign.com/download-medea-3.8>. The **Update from the Web** feature from the *MedeA Maintenance* program is **not** supported.

Updating *MedeA* will not affect any of your saved jobs, settings, results, structures, flowcharts, *license.txt*, *.options files, queueing scripts such as *PBS.tcl*, and any other user data. If you would like to backup your jobs, backup the following:

- The *Jobs* folder which is in *MD/2.0* by default for *MedeA* 3.0 and older and *MD* for *MedeA* 3.1 and newer
- *MDJobs.db* in *MD/Databases*

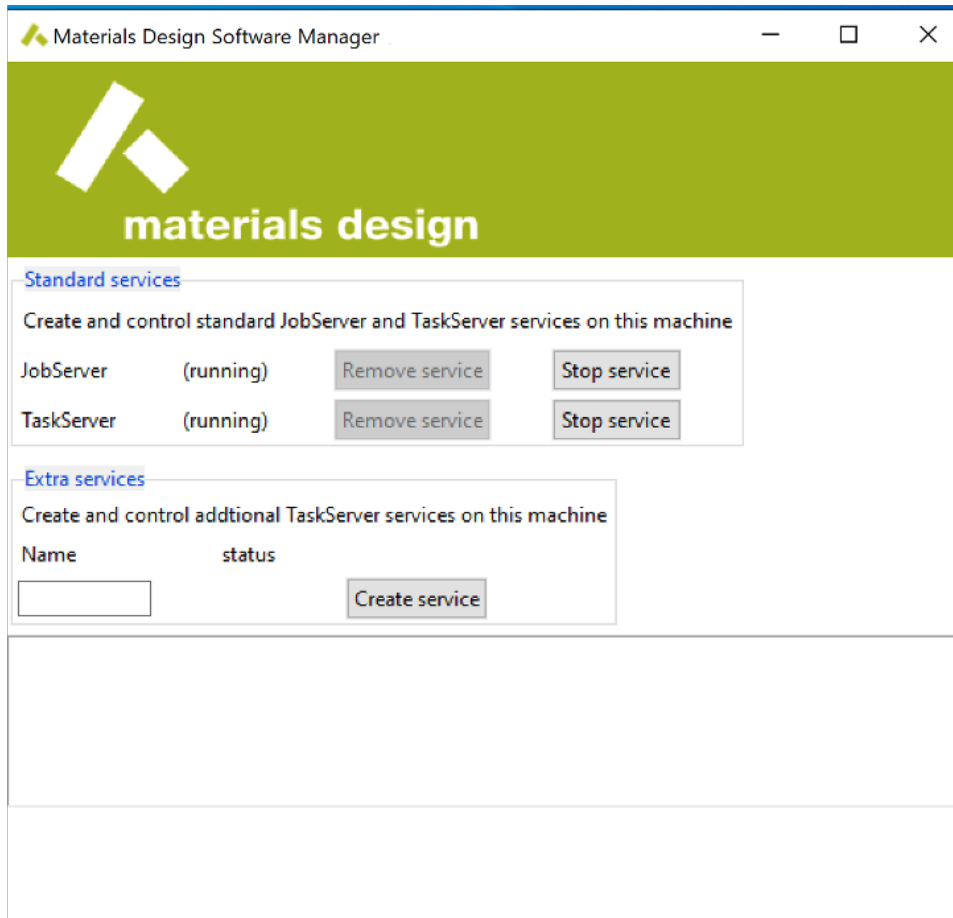
Warning: *MedeA* 3.8 requires an updated license from MD Support. Your licenses for *MedeA* 3.4, 3.3, 3.2, 3.1, 3.0, 2.22, and previous versions will not work for version 3.8 or future versions! If you are on maintenance, please send your license parameters to support@materialsdesign.com. **If you have licenses for *MedeA* 3.2, 3.1, 3.0, 2.22, or previous versions and your maintenance expired, updating to *MedeA* 3.8 would result in your *MedeA* to stop working!**

Since *MedeA* 3.1 the *2.0* folder is deprecated. All content of the *2.0* folder is moved one directory up to the root installation directory of *MedeA*, e.g. `C:\MD` or `~/MD`. That implies that in the update procedure the empty *2.0* folder will be removed.

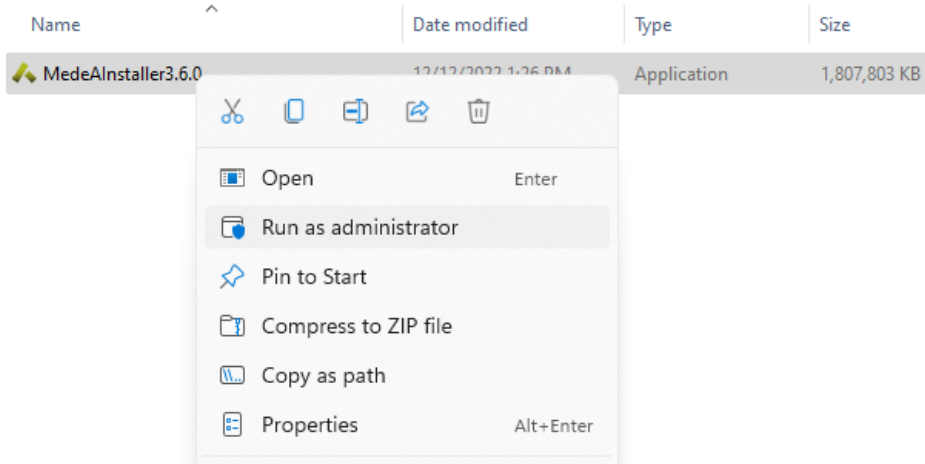
2 Update from the Windows Installer

Warning: Skip to the next section, *Update from ISO Image*, if you are updating from MedeA 3.0.X and older.

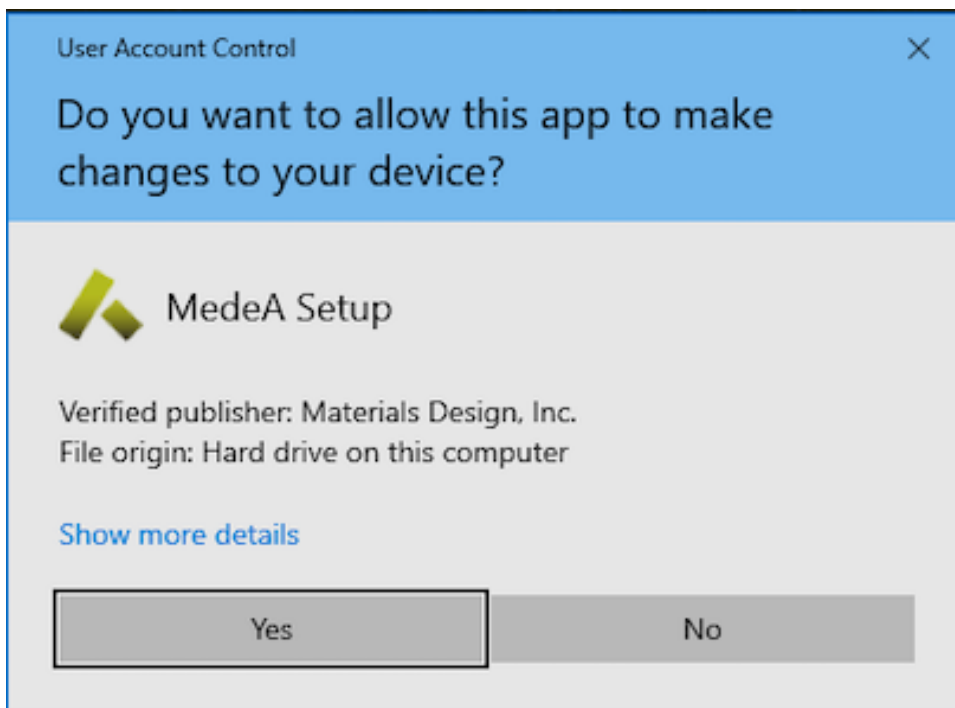
1. The first step is to stop the existing JobServer and TaskServer that are running. Go to the **Windows Start Menu >> Materials Design**, right-click on **MedeA Maintenance >> More >> Run as administrator**
2. Click **Manage MD Services**, and click **Stop service** buttons to stop the JobServer and TaskServer



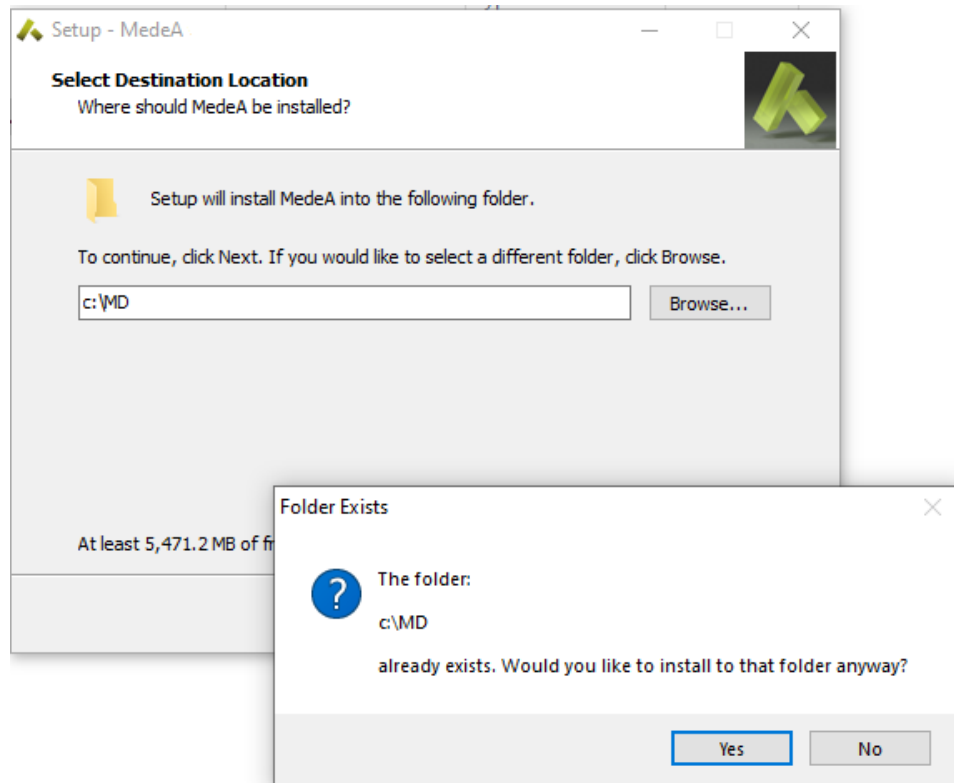
3. Click **Continue** to return to the home menu and click **Exit** again to close MDMaintenance
4. Go to the folder where you downloaded the *MedeAInstaller3.8.0.exe* Windows Installer, right-click and select **Run as administrator**



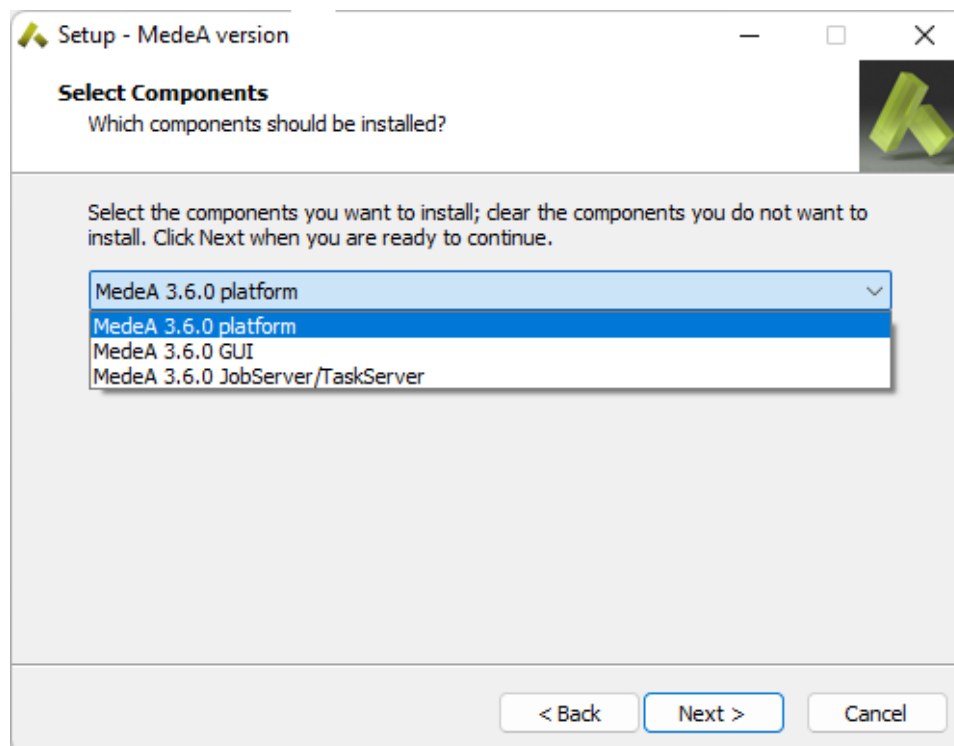
The installer is signed and verified to be from Materials Design, Inc.



5. Confirm the directory with the existing version of *MedeA*:



- Choose *MedeA 3.8.0 platform* to update the GUI, JobServer, and TaskServer. Click **Next**

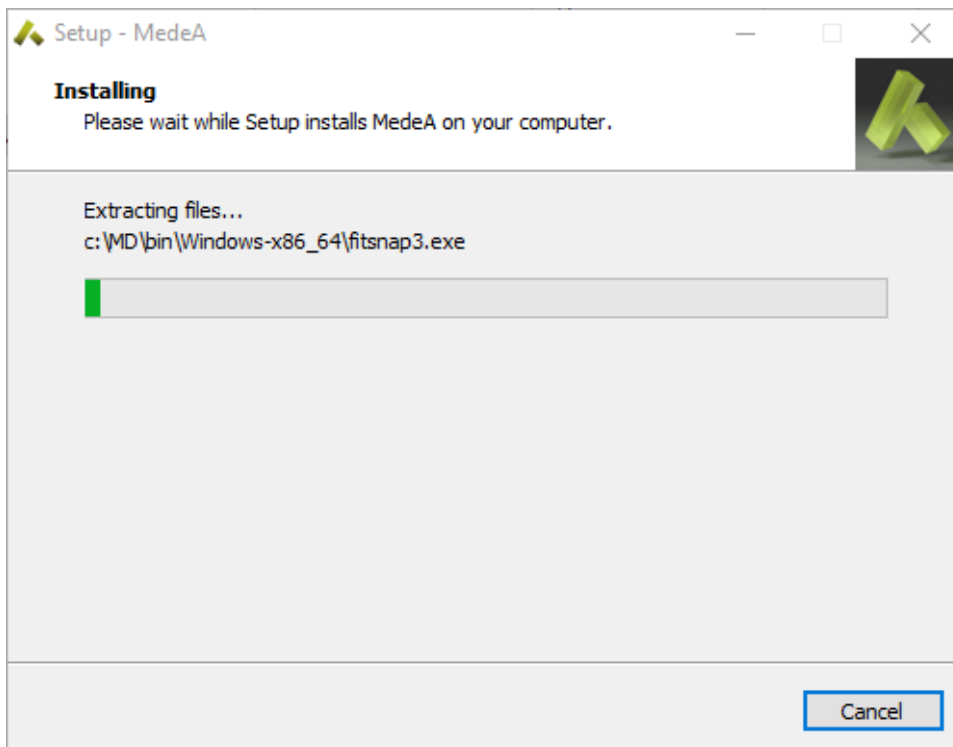


- Define the Start Menu folder name:

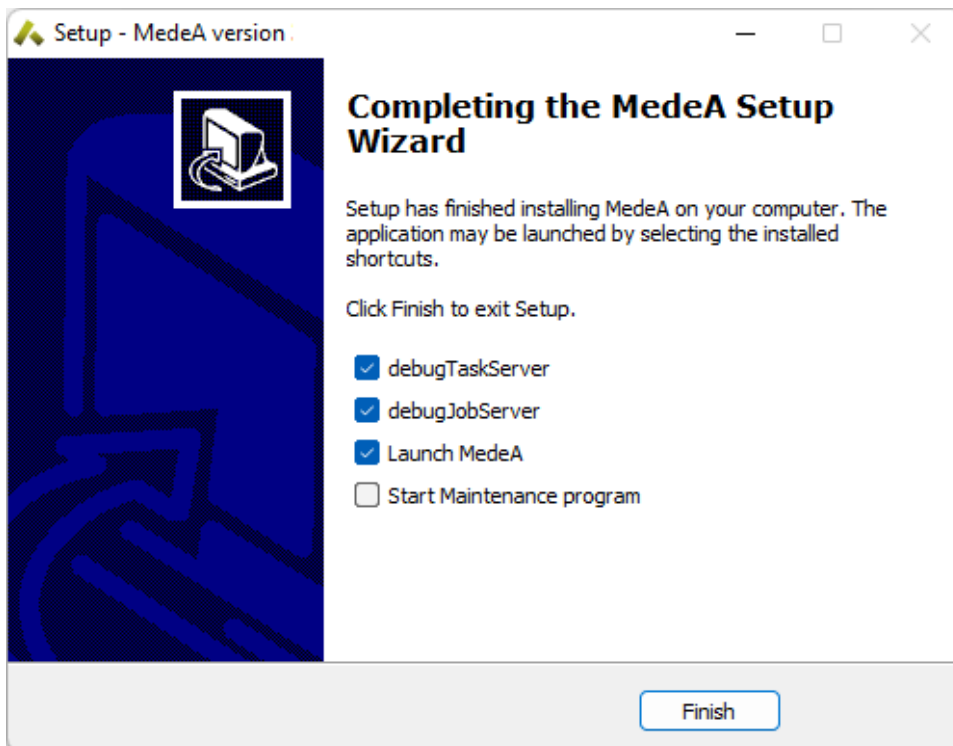
By default the folder is called *Materials Design* but you can change it to any other name such as *Materials Design 3*

- Click **Next** and proceed with the installation by following the prompted steps
- In the middle of the update, the installer asks whether to update the *MaterialsDesign.db* database.

The intention of the Materials Design database is to store custom structures, i.e. structures that you created. In case you stored structures in the Materials Design database, confirm with **No**. Confirm also with **No** in case you are uncertain. In case you never stored anything in the Materials Design database and you are sure, confirm with **Yes**.



10. Allow firewall access for the JobServer and TaskServer
11. The update process is complete. Launch MedeA and send MD support <support@materialsdesign.com> the new license parameters.



3 Update from ISO Image

With the ISO image, you can update *MedeA* from any version on Windows and Linux without having access to the Internet.

1. First step is to stop the existing JobServer and TaskServer that are running:

- On Windows, go to the **Windows Start Menu >> Materials Design**, right-click on **MedeA Maintenance >> More >> Run as administrator**
- On Linux, go to `<install_dir>/Linux-x86_64` and start MDMaintenance with sudo rights:

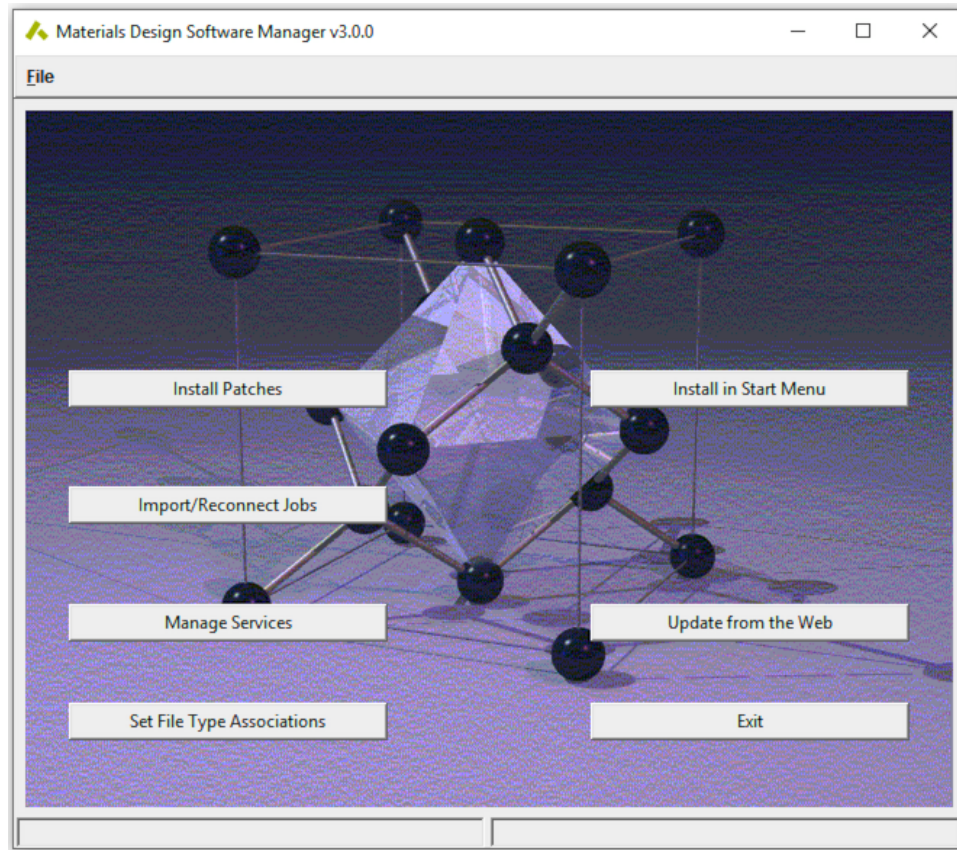
```
sudo ./MDMaintenance
```

- With MedeA 3.1.0 and newer:



(a) Click **Manage MD Services** and the **Stop Service** buttons to stop the JobServer and TaskServer.

- With MedeA 3.0.X and older:

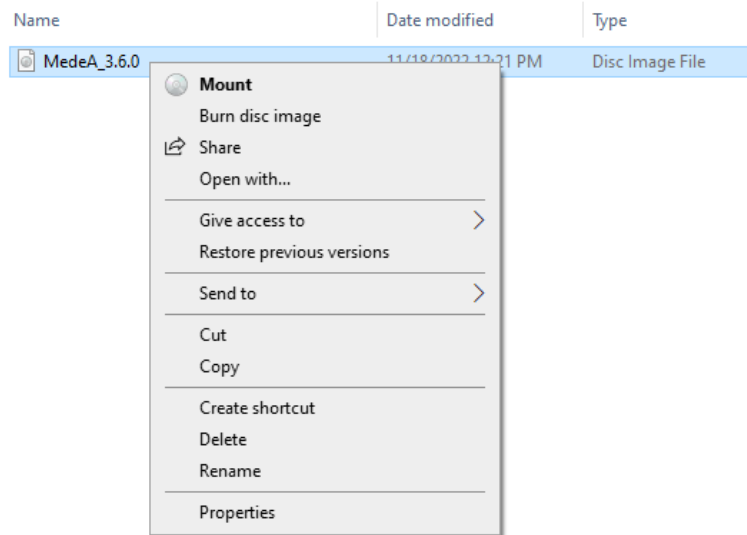


- (a) Click **Manage Services** on Windows and **Manage Daemons** on Linux.
- (b) Click **Stop Service** buttons to stop the JobServer and TaskServer.
- (c) Exit MDMaintenance.

3.1 Mounting the ISO Image on Windows

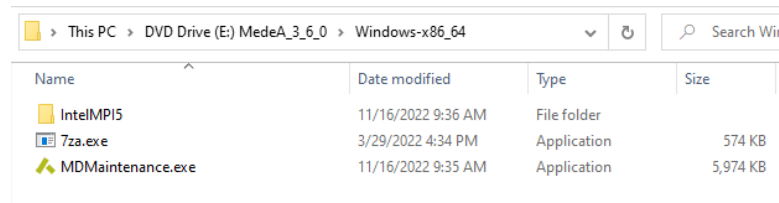
Warning: Windows does not support mounting ISO images from a shared drive (including Dropbox and virtual machine's shared folders). Therefore, please copy the ISO image to the Windows computer's local drive.

1. Go to the folder where you saved the downloaded ISO image. On Windows 8 or Windows 10, right-click on the ISO file and select **Mount** mounts the ISO image:

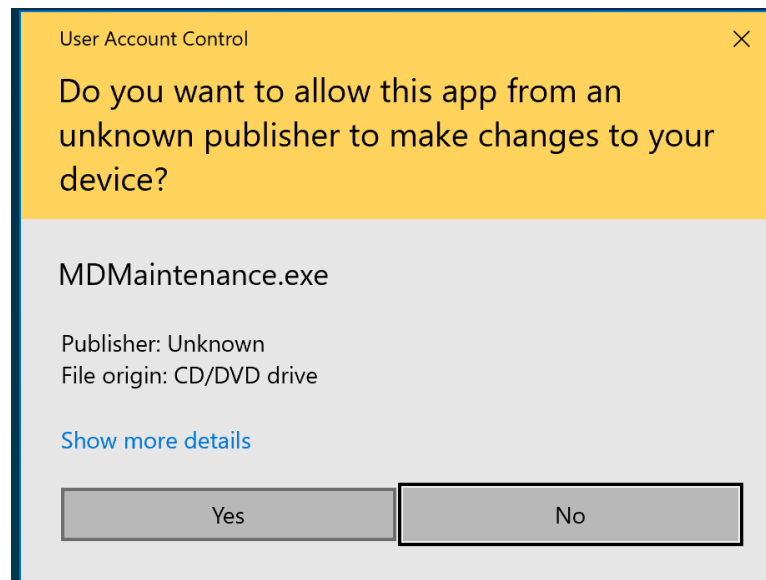


Hint: If you are experiencing any problems with mounting the ISO image on Windows with its native **Mount**, we recommend using [WinCDEmu \[1\]](#)

2. Open the mounted drive, *DVD Drive (E:)* in the example below, and right-click on *MDMaintenance* >> **Run as administrator** :



Click **Yes** to proceed with the installation as a standard user but with administration rights:



3.2 Mounting the ISO Image on Linux

[1] <https://wincdemu.sysprogs.org/download>

Note: *MedeA* and its graphical installer, MDMaintenance, work well with X11 display server but not with Wayland display server. Please log out and select X11 upon logging back in.

1. Use an existing directory or create a directory for the mounted drive, e.g.:

```
sudo mkdir -p /media/medea
```

2. Mount the ISO image as a loop device:

```
sudo mount -o loop MedeA_3.8.0.iso /media/medea
```

3. Open the mounted drive, move to the `Linux-x64_64` directory, and start MDMaintenance **without** sudo rights:

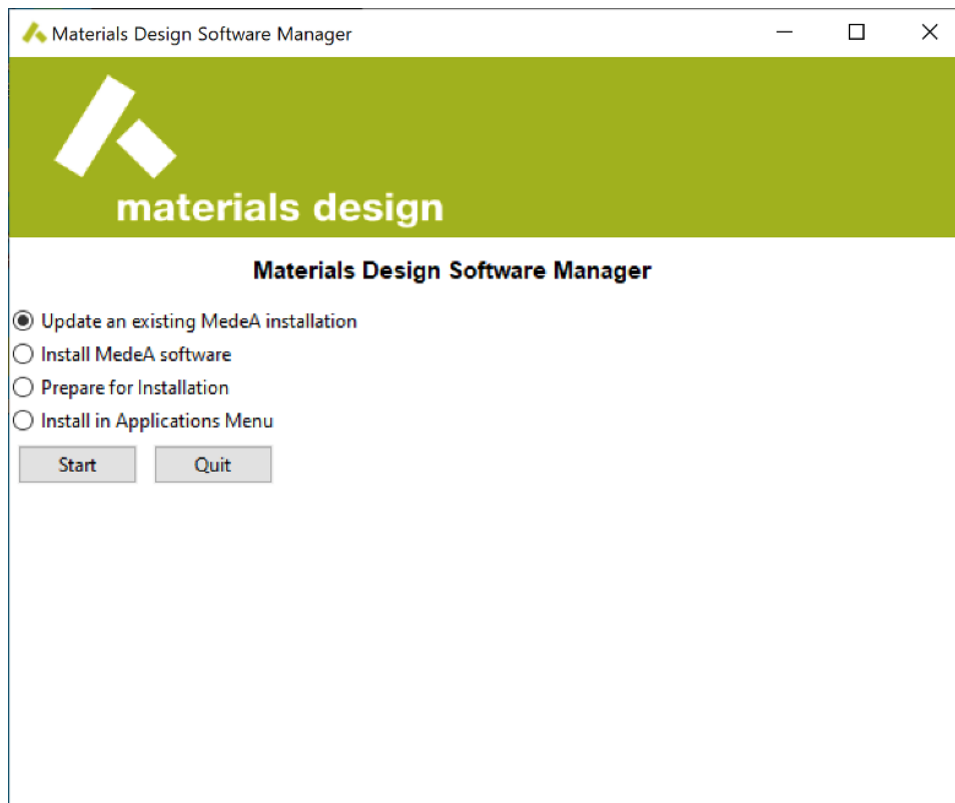
```
cd /media/medea/Linux-x86_64
./MDMaintenance
```

Note: *MedeA* on Windows and Linux look and behave the same way. So, unlike many Linux programs, the entire *MedeA* distribution is in one folder, including databases, executables and generated results. The location of temporary files can be changed any time; the best place is to install in a directory owned by the actual *medea* user or group.

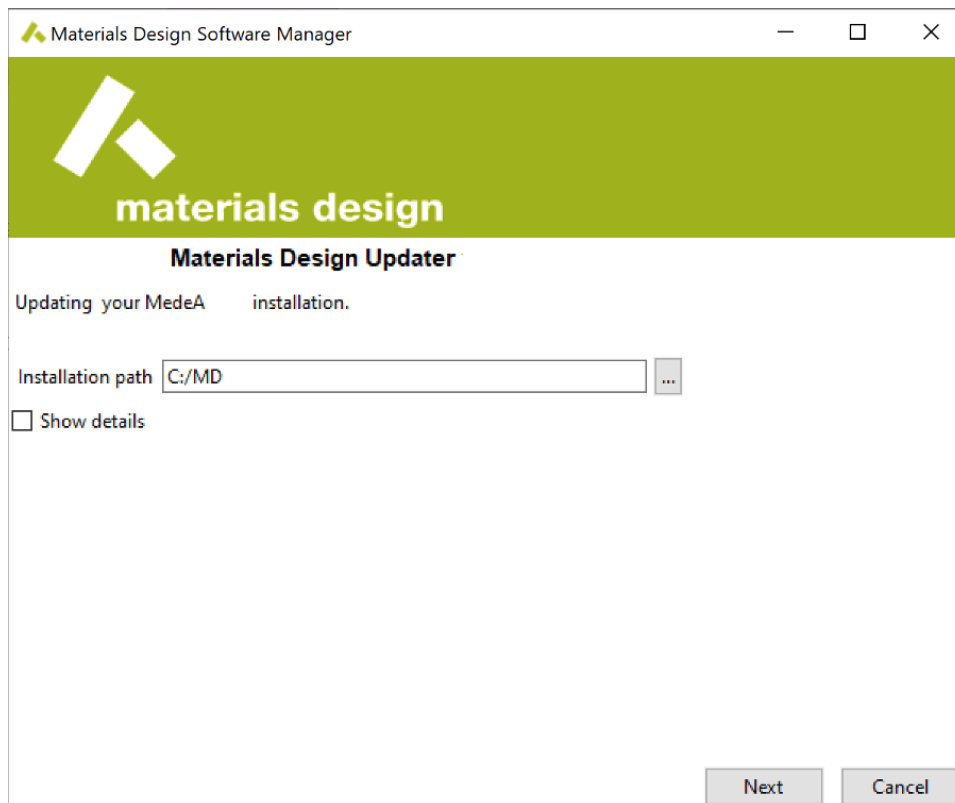
3.3 Updating *MedeA* on Windows and Linux

Despite some subtle differences in paths and directories, updating process on Windows and Linux are mostly the same.

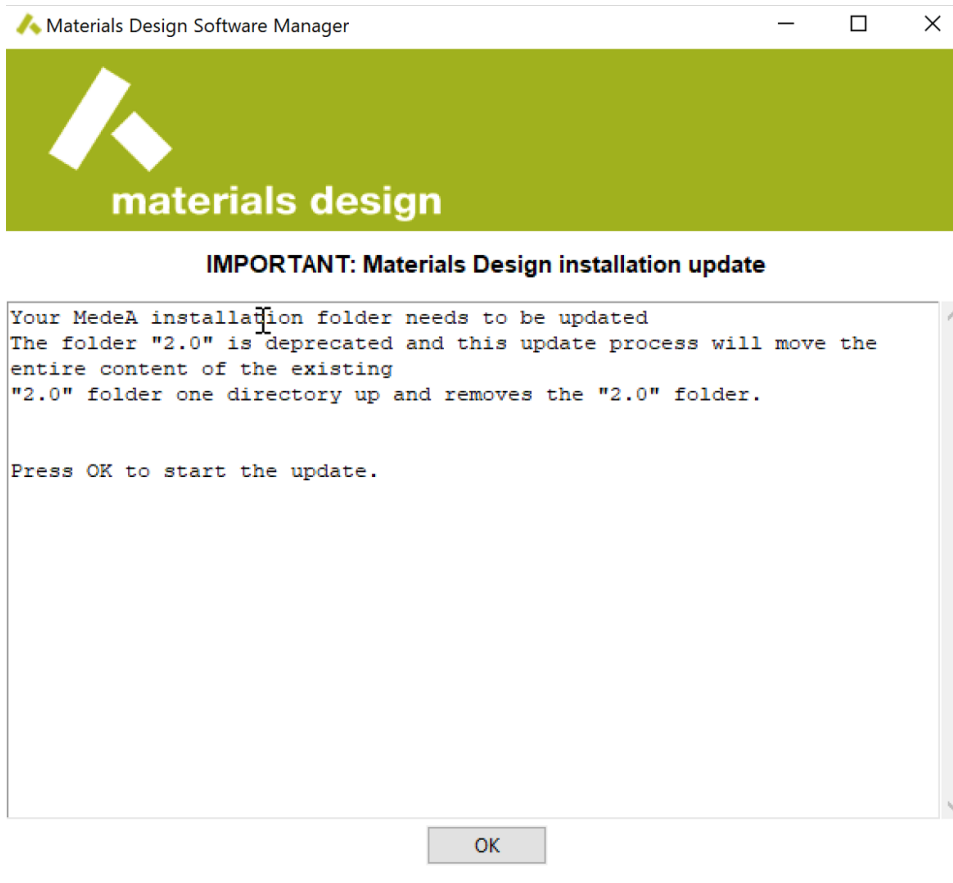
1. The *Materials Design Software Manager* window appears. Choose the option **Update an existing MedeA installation** and click **Start** :



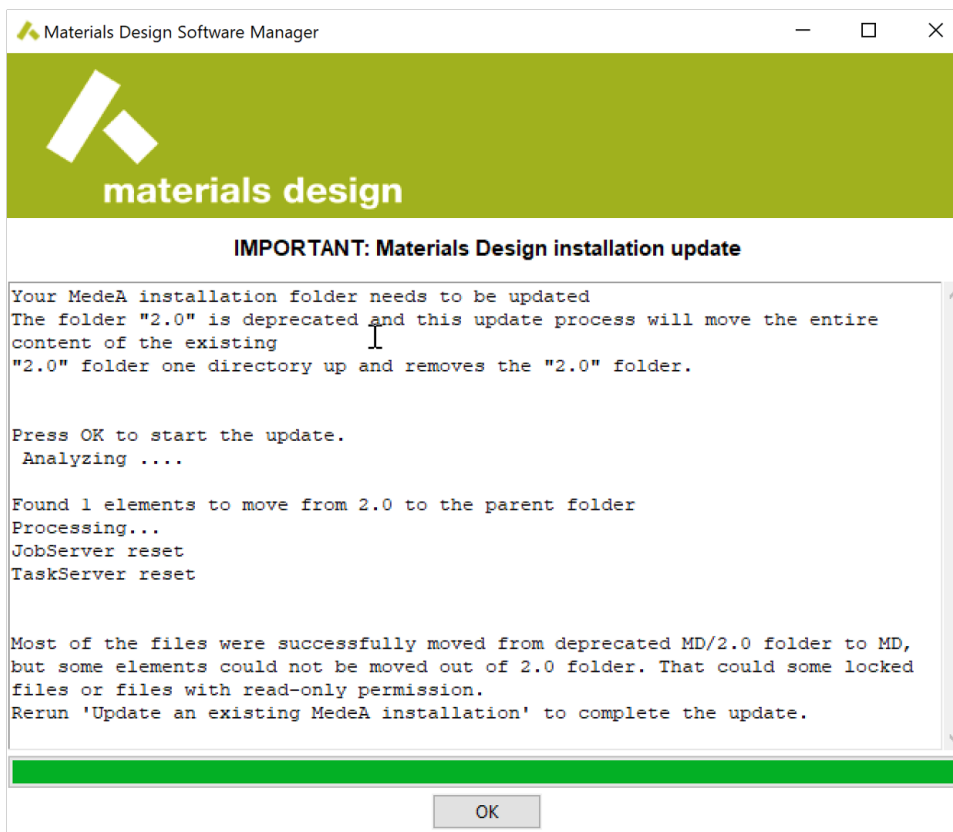
2. If updating from MedeA 3.1.0 or newer, skip to step 6. If updating from MedeA 3.0 or older, continue with step 3.
3. The 2.0 folder is deprecated. Set the *Installation path* to the current installation directory:



In the update process, all content of the 2.0 folder will be moved one directory up. As the last step the empty 2.0 folder will be removed. Click **OK** to proceed:



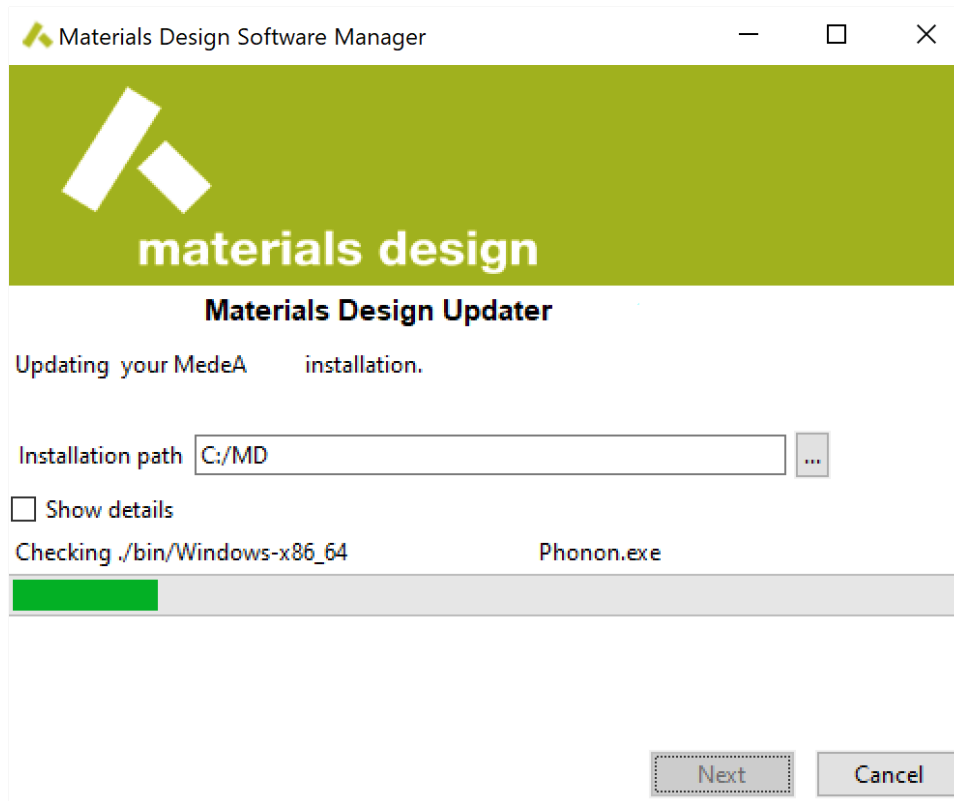
- Once the previous step is completed, the installer will wait for your **OK** to restart MDMaintenance:



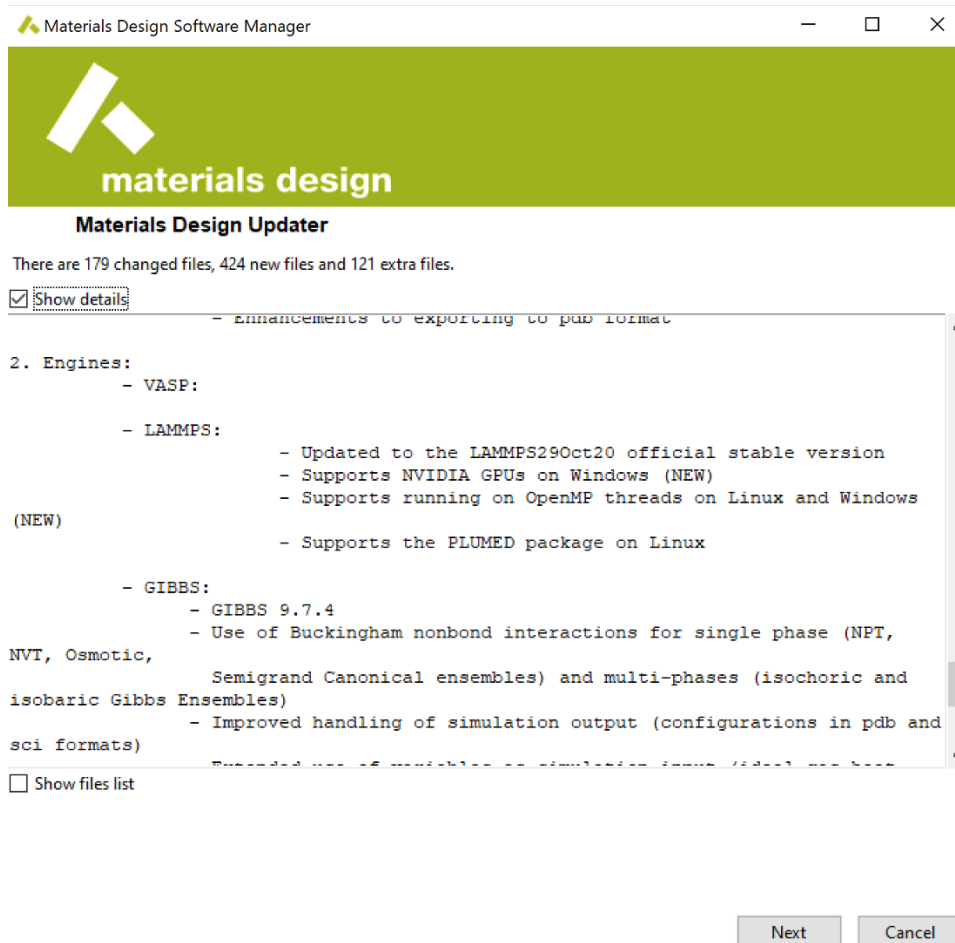
If MDMaintenance does not restart automatically, click **Quit** to close the current instance of MDMain-

tenance. To continue, start the MDMaintenance program with administrator rights.

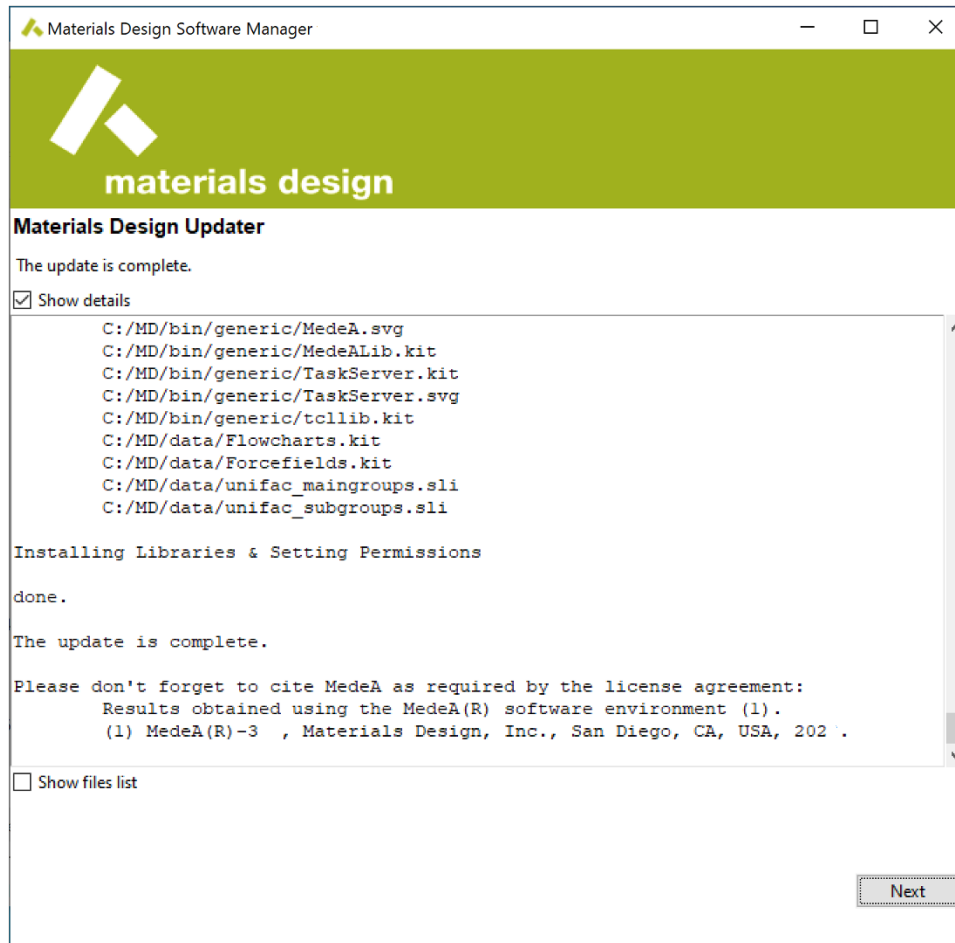
5. After MDMaintenance is restarted choose the option **Update an existing MedeA installation** and click **Start**
6. Choose the directory where you have the *MedeA* installed, click **Next** and MDMaintenance starts the checking process:



7. After the checking step, click **Next** to proceed with the update.

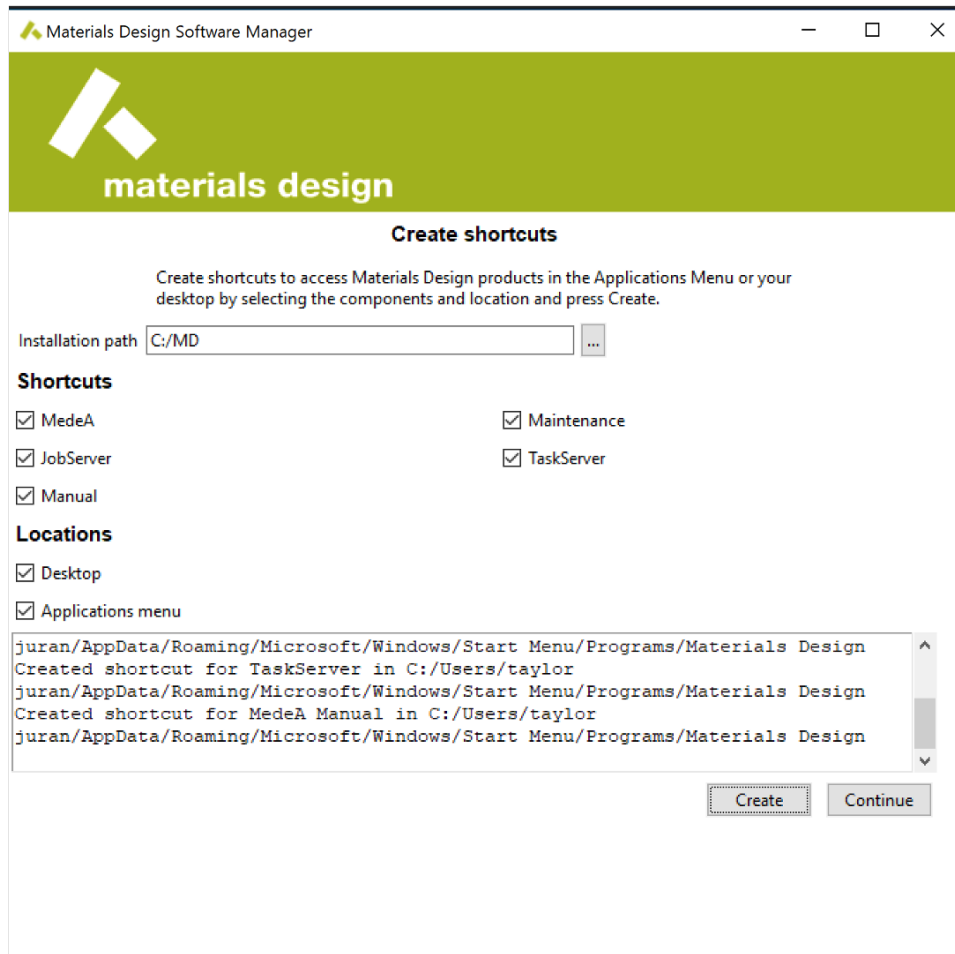


8. Click **Next** to finish the update:



Hint: Click **Show details** to see the list of changes and citation information

9. This returns to the main menu of the *Materials Design Software Manager* window. Choose **Install in Application Menu** and click **Start** to install menu shortcuts and icons in the desktop and the application menu. Make your selections and click **Create** :



Click **Continue** to exit and then **Quit**

10. On Windows, this is the last step: use the newly created/updated MDMaintenance from the desktop or the application menu (**Materials Design** menu) to start MDMaintenance as administrator and start the JobServer and TaskServer with the **Start service** buttons.
 - If the JobServer and TaskServer web pages at <http://localhost:32000> and <http://localhost:23000>, respectively, are still of the 3.0 version, start MDMaintenance again and follow steps 2-5 below to remove and re-create the JobServer and TaskServer services.

11. On Linux, since the JobServer and TaskServer service scripts are moved from the directory `/etc/init.d` to the directory `/etc/systemd/system`, there is one additional step to re-create the JobServer and TaskServer services:

- (a) Start MDMaintenance from the **installation directory** (e.g. `/home/<username>/MD/Linux-x86_64`) **without** sudo rights

```
./MDMaintenance.x
```

- (b) Check **Manage MD service** and click **Start**
- (c) Enter your admin/sudo password in the *Sudo password* box and click **Check**
- (d) Click the **Remove service** buttons for both the JobServer and the TaskServer
- (e) Click the **Create service** buttons to re-create the services

Hint: When any of the TaskServers do not start after the above steps, make sure the `MD/TaskServer` directory is fully owned by the user who started MDMaintenance:

```
sudo chown <username> -R /home/<username>/MD/TaskServer
```

12. The *MedeA* update has been completed and skip to the last section *After Updating to 3.8*

4 Update from the Materials Design Update Server

Warning: Update from the Web is not supported if you are updating from older versions of *MedeA* (3.0, 2.22, and older) to 3.8, please refer to the previous sections on updating to 3.8 with the Windows Installer or ISO images.

If you have installed or updated to *MedeA* 3.1.0 or newer via the Windows Installer or ISO images, you can then use the **Update from the Web** option in MDMaintenance to update to newer versions of *MedeA*, including point releases such as *MedeA* 3.1.2 or new major releases such as *MedeA* 3.8.

To update from the Materials Design Update Server via the internet, you will need a username and password (credentials) to access the server. If you haven't received credentials yet, send an email to [MD Support \[2\]](mailto:MD_Support@materialsdesign.com) to receive the updated credentials. You can always retrieve or change your password at [my.materialsdesign.com/user/password \[3\]](http://my.materialsdesign.com/user/password), provided you are not signed in.

1. The first step is to stop every running JobServer and TaskServer.

- On Windows, start MDMaintenance as administrator: **Windows Start Menu >> Materials Design**, right-click on **MD Maintenance >> More >> Run as administrator**
- On Linux, change to the directory `<install_dir>/Linux-x86.64` and start MDMaintenance with sudo rights:

```
sudo ./MDMaintenance
```

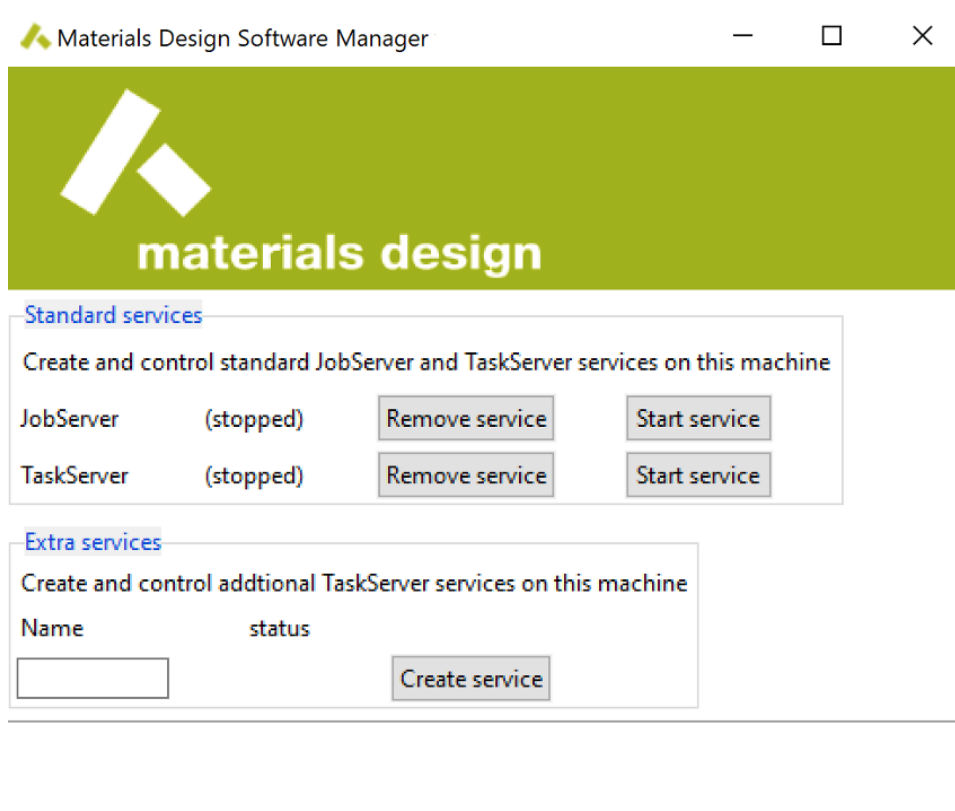
Note: Start MDMaintenance with administrator rights to stop the JobServer and TaskServer services

[2] support@materialsdesign.com

[3] <http://my.materialsdesign.com/user/password>

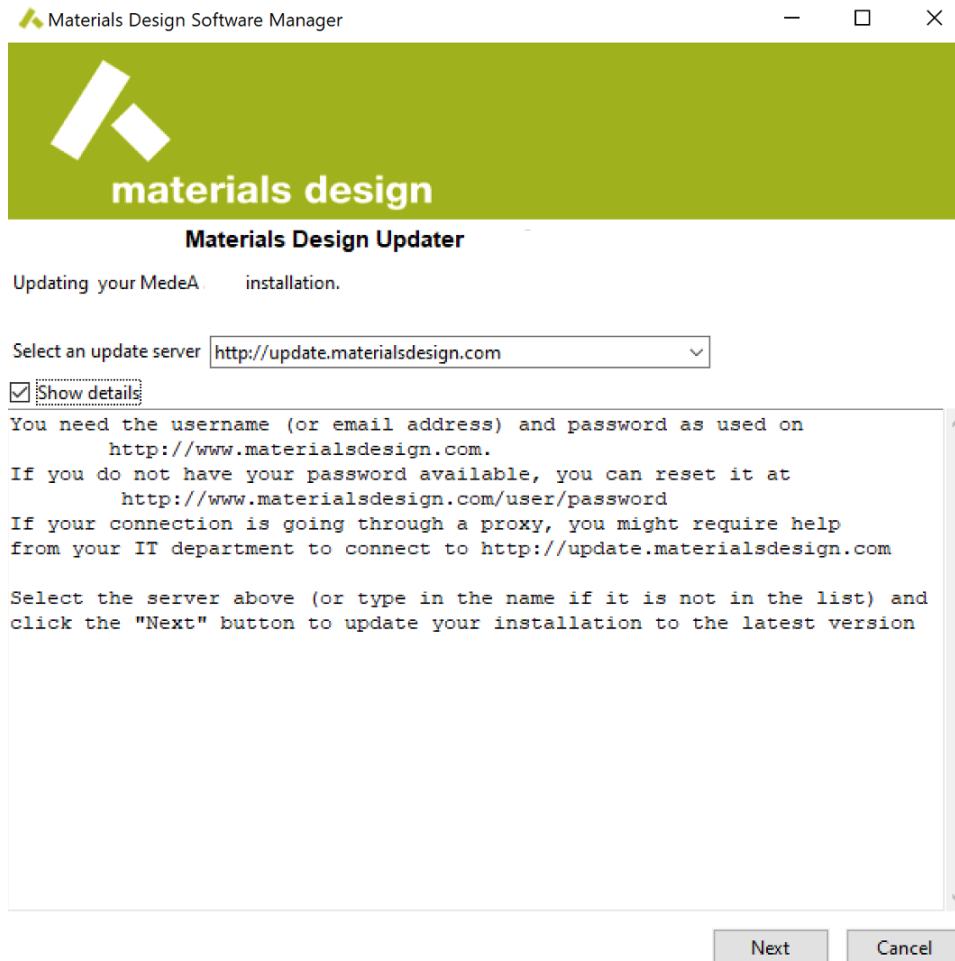


2. Click **Manage MD services** , click **Stop service** buttons to stop the JobServer and TaskServer.
3. Click **Continue** to go back to the home menu:

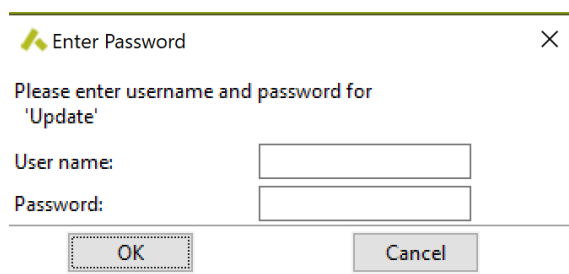


4. In the *MedeA* Software manager mark the checkbox of the option **Update from the Web** and confirm with **Start** .

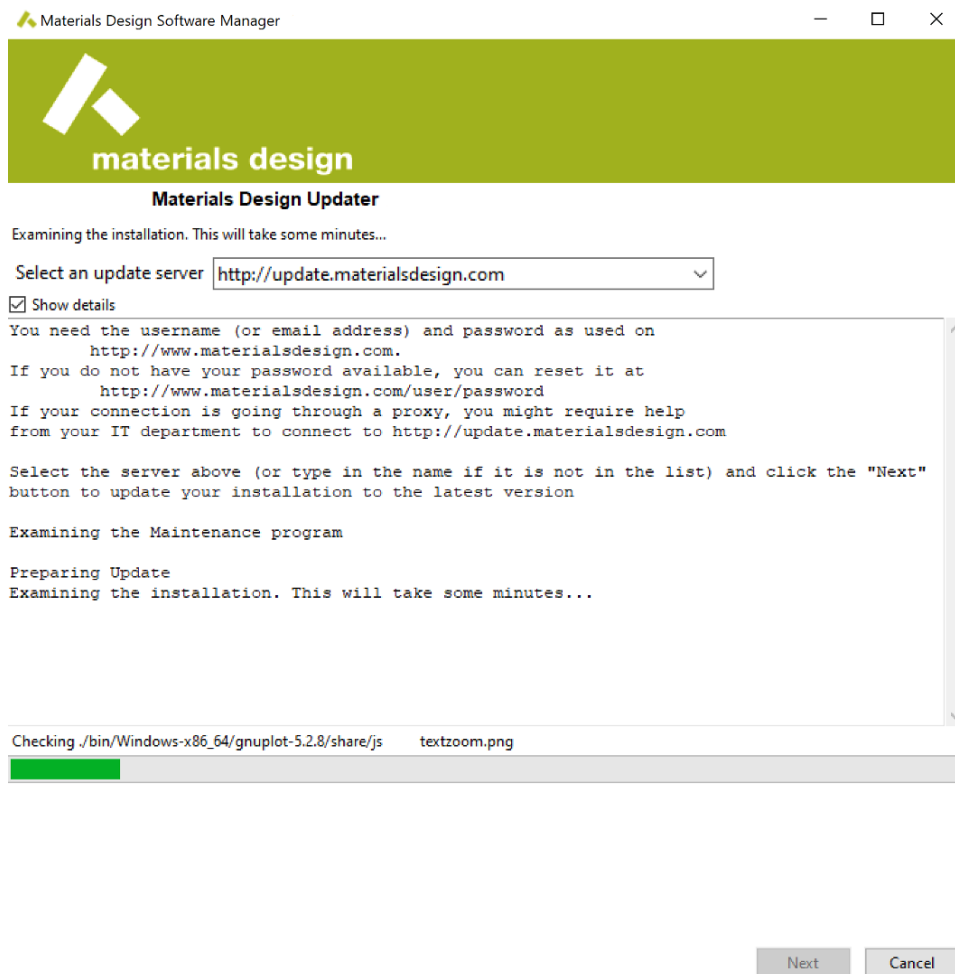
5. Ensure the *Select an update server* box is `http://update.materialsdesign.com` and click on **Next** to continue.



6. In the appearing prompt enter as Username your Materials Design user-ID or email address and provide your Materials Design password, then click **OK**.



7. The Updater will restart to update MDMaintenance itself. Click **Yes** to continue.
8. After MDMaintenance restarted, click **Update from the Web** to repeat steps 4-6.
9. MDMaintenance will first perform an analysis to determine the necessary changes. Click the **Next** button.



10. The update will start and necessary changes will be downloaded from the update server to your local copy.
11. After the update finished, click the **Next** button to exit.

Your *MedeA* installation has been updated to a newer point release, e.g., *MedeA* 3.1.2, or a new major release, e.g., *MedeA* 3.8. In case of the point release, your 3.1 license will still work so you would not need to request a new license. However, if you have updated to 3.8, you would need to request a new license from MD Support [4]

5 Update on Linux on the Command-Line

Whenever possible, please update *MedeA* with the graphical user interface, and the option to update *MedeA* on the command-line is experimental and should be reserved for administrator staff and experienced users.

5.1 Stopping and Removing Existing JobServer and TaskServer Services

1. Stop the existing JobServer and TaskServer
 - With *MedeA* 3.0 and older (2.22, 2.21, etc):

```
sudo /etc/init.d/mdjobserver stop
sudo /etc/init.d/mdtaskserver stop
```

- With *MedeA* 3.1 and newer:

[4] support@materialsdesign.com

```
sudo systemctl stop mdjobserver.service
sudo systemctl stop mdtaskserver.service
```

2. In *MedeA* 3.0 and older (2.22, 2.21, etc), remove the JobServer and TaskServer service scripts:

```
sudo rm -rf /etc/init.d/mdjobserver
sudo rm -rf /etc/init.d/mdtaskserver
```

5.2 Mounting the ISO Image on Linux

1. Use an existing directory or create a directory for the mounted drive, e.g.:

```
sudo mkdir -p /media/medea
```

2. Mount the ISO image as a loop device:

```
sudo mount -o loop MedeA_3.8.0.iso /media/medea
```

5.3 Performing the Update on the Command Line

1. Move to the mounted drive, change to the `Linux-x64_64` directory, and start MDMaintenance **without** sudo rights:

```
cd /media/medea/Linux-x86_64
./MDMaintenance -update
```

Hint: You can use `./MDMaintenance -help` to show a list of options

2. Choose the existing directory to update:

```
Welcome to the Materials Design Updater 3.8.0
Update directory [/home/medea/MD]:
```

3. Hit return/enter and follow the prompt. The updater will first move the content of the 2.0 folder one directory up, and update *MedeA*.

4. Update of the *MedeA* core components is complete:

```
Installing Libraries & Setting Permissions
done.

The update is complete.

Please don't forget to cite MedeA as required by the license agreement:
Results obtained using the MedeA(R) software environment (1).
(1) MedeA(R)-3.8, Materials Design, Inc., San Diego, CA, USA, 2023.
```

5. Next we will create the JobServer and TaskServer. Change to the **updated installation directory**, e.g., `/home/<username>/MD/Linux-x86_64` and enter:

```
sudo ./MDMaintenance.x -createjobserver
sudo ./MDMaintenance.x -createtaskserver
```

The JobServer and TaskServer scripts are created in the `/etc/systemd/system` directory.

6. Start the JobServer and TaskServer

```
sudo systemctl start mdjobserver.service
sudo systemctl start mdtaskserver.service
```

You can use the following commands to check the status of the services:

```
sudo systemctl status mdjobserver.service
sudo systemctl status mdtaskserver.service
```

or

```
wget localhost:32000
wget localhost:23000
```

7. Finish the update

6 After the Update

1. Check if the JobServer and TaskServer are updated to 3.8 and up and running. See [Checking, Starting, and Stopping JobServer and TaskServer](#) for more details.
2. Open *MedeA* GUI and send the new license parameters to [MD Support](#) [5]

[5] support@materialsdesign.com