

# **Updating an Existing MedeA Installation**

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# **1** Introduction

This section describes the procedure to update your existing *MedeA* installation to *MedeA* 3.9. 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 3.9 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 3.9 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* 3.9 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 3.9 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* 3.9 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  $^{\sim}$ /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

🙏 Materials [	Design Software N	lanager		_	×
, in the second	haterials	s design			
Standard serv	ices				
Create and co	ntrol standard Job	Server and TaskServer se	rvices on this machine	2	
JobServer	(running)	Remove service	Stop service		
TaskServer	(running)	Remove service	Stop service		
Extra services Create and co	ntrol addtional Tas	kServer services on this	machine		
Name	status	Create service			

- 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 *MedeAInstaller3.9.0.exe* Windows Installer, right-click and select **Run as administrator**



Name	^	Date modif	fied	Туре	Size
ሉ MedeAlnstaller3.6.0		12/12/2022	1.26 DM	Application	1,807,803 KB
	% O ED	i 🖸			
	Open		Enter		
	📑 Run as admir	nistrator			
	🔗 Pin to Start				
	Compress to	ZIP file			
	🛄 Copy as path	n			
	E Properties		Alt+Enter		

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

User Account Control	×
Do you want to allow this app to make changes to your device?	
人 MedeA Setup	
Verified publisher: Materials Design, Inc. File origin: Hard drive on this computer	
Show more details	
Yes No	

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



, Setup - MedeA		—		
Select Destination Location			10	
Where should MedeA be installed	d?			
Setup will install MedeA	into the following folder.			
To continue, click Next. If you w	ould like to select a different fo	der, click Bro	wse.	
c: WD		Br	owse	
Folder	Exists			×
Folder At least 5,471.2 MB of fr	Exists			×
Folder At least 5,471.2 MB of fr	Exists The folder:			×
Folder At least 5,471.2 MB of fr	The folder:			×
Folder At least 5,471.2 MB of fr	Exists The folder: c:\MD already exists. Would yo	u like to insi	tall to that folder a	anyway?
Folder At least 5,471.2 MB of fr	Exists The folder: c:\MD already exists. Would yo	u like to insi	tall to that folder a	× anyway?

6. Choose MedeA 3.9.0 platform to update the GUI, JobServer, and TaskServer. Click Next

ሉ Setup - MedeA version	_		$\times$
Select Components Which components should be installed?			
Select the components you want to install; clear the compo install. Click Next when you are ready to continue.	nents you do no	ot want to	
MedeA 3.6.0 platform		~	· ]
MedeA 3.6.0 platform MedeA 3.6.0 GUI MedeA 3.6.0 JobServer/TaskServer			
< Back	Next >	Can	cel

7. 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* 

- 8. Click Next and proceed with the installation by following the prompted steps
- 9. 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.

🔥 Setup - MedeA	—		$\times$
Installing Please wait while Setup installs MedeA on your computer.			
Extracting files c: \MD\bin\Windows-x86_64\fitsnap3.exe 			
		Can	icel

- 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.

ሉ Setup - MedeA version	_	×
	Completing the MedeA Setup Wizard	
	Setup has finished installing MedeA on your computer. The application may be launched by selecting the installed shortcuts.	
	Click Finish to exit Setup.	
	debugTaskServer	
	debugJobServer	
	Launch MedeA	
	Start Maintenance program	
	Finish	



# **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:

• With MedeA 3.1.0 and newer:

Materials design         Materials Design Software Manager         Update from the Web         Manage MD services         Import Jobs         Personent lebs	
Materials design         Materials Design Software Manager         Update from the Web         Manage MD services         Import Jobs         Personent lebs	
Materials Design Software Manager Update from the Web Manage MD services Import Jobs Researce to be	
Materials Design Software Manager Update from the Web Manage MD services Import Jobs	
Update from the Web Manage MD services Import Jobs	
Manage MD services Import Jobs	
Import Jobs	
Pasannast Jaha	
Reconnect Jobs	
Install in Applications Menu	
Set File Type Associations	
Start Quit	

- (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:



Name		Date modified	Туре
Name	Image: Share         Open with         Give access to         Restore previous versions         Send to	Date modified	Type Disc Image File
	Cut Copy Create shortcut Delete Rename Properties		

**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 :

→ This PC → DVD Drive (E:) Mede	A_3_6_0 > Windows-x86_64	5 V	🔎 Search Wir
Name	Date modified	Туре	Size
IntelMPI5	11/16/2022 9:36 AM	File folder	
📧 7za.exe	3/29/2022 4:34 PM	Application 574	
🙏 MDMaintenance.exe	11/16/2022 9:35 AM	Application	5,974 KB

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



### 3.2 Mounting the ISO Image on Linux

<sup>[1]</sup> 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\_3.9.0.iso /media/medea

3. Open the mounted drive, move to the Linux-x86\_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:

🔥 Materials Design Software Manager	_	×
materials design		
Materials Design Updater		
Updating your MedeA installation.		
Installation with Cr/MD		

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:

🙏 Materials Design Software Manager	_		×
materials design			
IMPORTANT: Materials Design installation update	e		
Your MedeA installation folder needs to be updated The folder "2.0" is deprecated and this update process will entire content of the existing "2.0" folder one directory up and removes the "2.0" folder	l move	the	^
Press OK to start the update.			

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

OK



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:

ㅅ Materials Design Software Manager	—		×
materials design			
Materials Design Updater			
Updating your MedeA installation.			
Installation path C:/MD			
Checking ./bin/Windows-x86_64 Phonon.exe			
	Next	Ca	ncel

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

٨ Materials Design Software Manager	- 0	×
materials design		
Materials Design Updater		
There are 179 changed files, 424 new files and 121 extra files.		
Show details - Ennancements to exporting to publicimat		^
2. Engines: - VASP:		
- LAMMPS:		
- Updated to the LAMMPS29Oct20 offic - Supports NVIDIA GPUs on Windows () - Supports running on OpenMP threads (NEW)	ial stable version NEW) 9 on Linux and Windows	
- Supports the PLUMED package on Lin	ıux	
- GIBBS: - GIBBS 9.7.4 - Use of Buckingham nonbond interactions fo:	single phase (NPT,	
NVT, Osmotic,	· ·	
Semigrand Canonical ensembles) and multi-	hases (isochoric and	
- Improved handling of simulation output (c	onfigurations in pdb an	ıd
sci formats)	-	
Show files list		

Next Cancel

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 dekstop and the application menu. Make your selections and click **Create** :

🔥 Materials Design Software Manager	-		×
materials design			
Create shortcuts			
Create shortcuts to access Materials Design products in the Applications Menu or your desktop by selecting the components and location and press Create.			
Installation path C:/MD			
Shortcuts			
MedeA Maintenance			
☑ JobServer ☑ TaskServer			
Manual			
Locations			
☑ Desktop			
Applications menu			
juran/AppData/Roaming/Microsoft/Windows/Start Menu/Programs/Materials Created shortcut for TaskServer in C:/Users/taylor juran/AppData/Roaming/Microsoft/Windows/Start Menu/Programs/Materials Created shortcut for MedeA Manual in C:/Users/taylor juran/AppData/Roaming/Microsoft/Windows/Start Menu/Programs/Materials	Desig Desig	yn yn yn	<b>^</b>
Create	(	Continue	e

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 Job-Server and TaskServer services:
  - (a) Start MDMaintenance from the **installation directory** (e.g. /home/<username>/MD/Linuxx86\_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 3.9

### 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 3.9, please refer to the previous sections on updating to 3.9 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* 3.9.

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] to receive the updated credentials. You can always retrieve or change your password at my.materialsdesign.com/user/password [3], 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

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

<sup>[2]</sup> support@materialsdesign.com



O Set File Type Associations

Start	Quit
-------	------

- 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:

\land Materials [	Design Software N	Manager	- 0	×
, n	haterial	s design		
Standard serv	ices			
Create and co	ntrol standard Joł	Server and TaskServer s	ervices on this machine	
JobServer	(stopped)	Remove service	Start service	
TaskServer	(stopped)	Remove service	Start service	
-Extra services				
Create and co	ntrol addtional Ta	skServer services on this	machine	
Name	status			
	]	Create service		

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.

ㅅ Materials Design Sof	ware Manager	—		×
mater	Ials design			
Updating your MedeA	installation.			
Select an update server	ttp://update.materialsdesign.com	~]		
Show details				
http://w http://w If your connectio from your IT depa Select the server click the "Next"	w.materialsdesign.com/user/password is going through a proxy, you might i ctment to connect to http://update.mate above (or type in the name if it is no putton to update your installation to t	require he erialsdesion ot in the i the latest	lp gn.com list) a versio	nd n
		Next		n col

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.

🙏 Enter Password		×
Please enter username an 'Update'	d password for	
User name:		
Password:		
ОК	Cancel	

- 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.

🔥 Materials Design Software Manager	-		×
materials design			
Materials Design Updater			
Examining the installation. This will take some minutes			
Select an update server http://update.materialsdesign.com 🗸			
Show details			
You need the username (or email address) and password as used on http://www.materialsdesign.com. If you do not have your password available, you can reset it at http://www.materialsdesign.com/user/password If your connection is going through a proxy, you might require help from your IT department to connect to http://update.materialsdesign.com			1
Select the server above (or type in the name if it is not in the list) and o button to update your installation to the latest version	click the	e "Nex	c"
Examining the Maintenance program			
Preparing Update Examining the installation. This will take some minutes			
Checking ./bin/Windows-x86_64/gnuplot-5.2.8/share/js textzoom.png			
_			
	Next	Ca	ncel

- 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* 3.9. 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 3.9, 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:

<sup>[4]</sup> 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_3.9.0.iso /media/medea
```

#### 5.3 Performing the Update on the Command Line

1. Move to the mounted drive, change to the Linux-x86\_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 3.9.0
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)-3.9, 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 3.9 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]

<sup>[5]</sup> support@materialsdesign.com