# Installing MedeA on Windows and Linux from ISO

## Contents

# 1  Introduction

This section goes over the steps of performing a fresh installation of *MedeA* on Windows and Linux, respectively, from a downloaded ISO image of the installation DVD.

**Note:**  This section is for a new installation of *MedeA* on a computer. For updating an existing *MedeA* version to 3.8 from the ISO image of the installation DVD, please see Section Update Existing MedeA.

On Windows, it is necessary to install *MedeA* with the graphical installer, while on Linux, there is an option to install only the JobServer and TaskServer **without** the graphical installer, that is, fully on the command-line.

**Note:**  Whenever possible, please install *MedeA* **with** the graphical user interface, and the option to install *MedeA* on the command-line is experimental and should be reserved for administrator staffs and experienced users to install **only** the JobServer and TaskServer.

# 2  Regular Installation with the Graphical Installer

Installing *MedeA* on Windows and Linux using the ISO image with the graphical Installer are very similar. The only differences lie in mounting the ISO image and starting MDMaintenance **with** and **without** administrator rights:

- On Windows, please start MDMaintenance **with** administrator rights
- On Linux, please start MDMaintenance **without** administrator rights

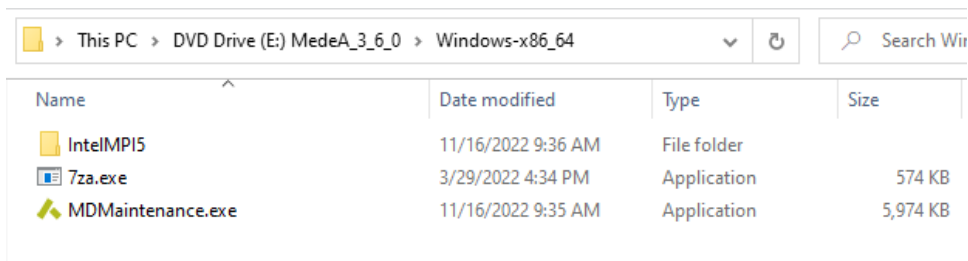## 2.1  Mounting the ISO image on Windows

**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  would mount the ISO image:
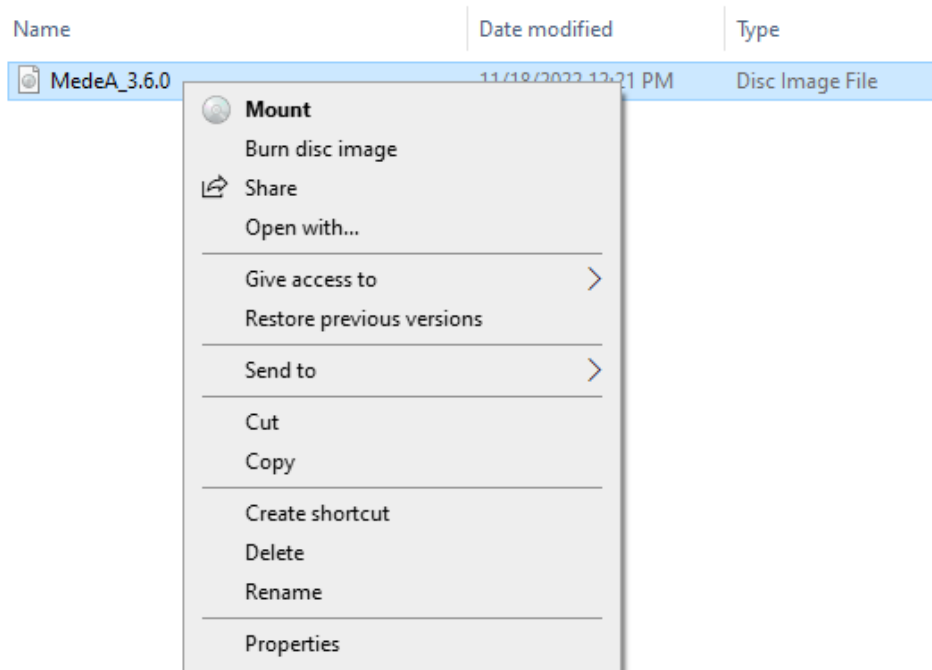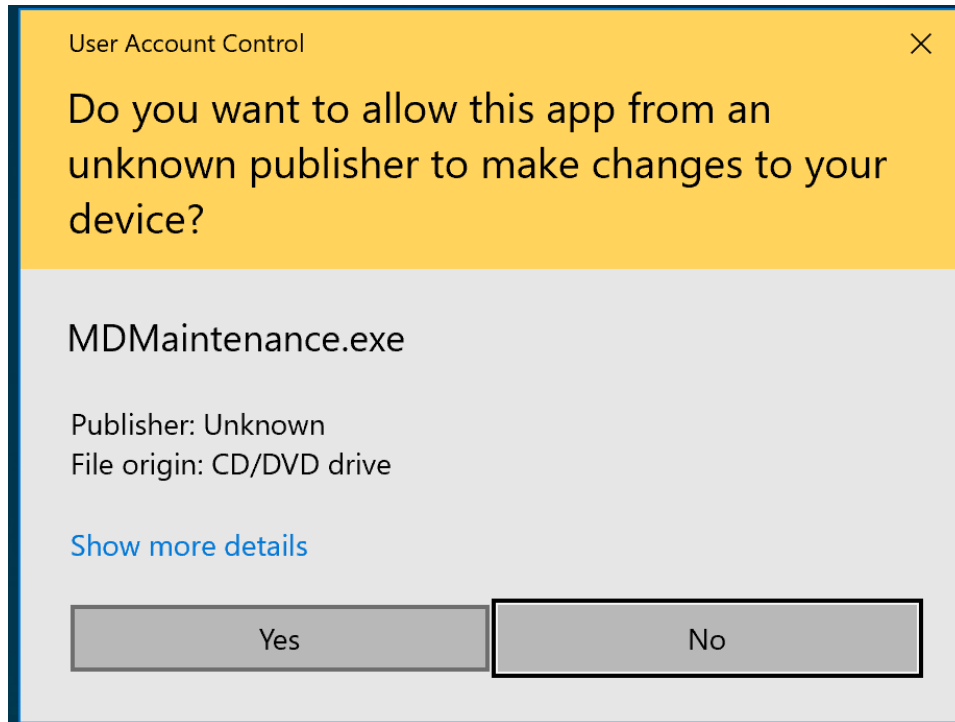


**Hint:** If you are experiencing any problems with mounting the ISO image on Windows with its native **Mount**, we recommend using WinCDEmu [1]

2. Go to 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:

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

User Account Control ☓

Do you want to allow this app from an
unknown publisher to make changes to your
device?

MDMaintenance.exe

Publisher: Unknown
File origin: CD/DVD drive

Show more details

| Yes | No |

## 2.2 Mounting the ISO image on Linux

**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. Before mounting the ISO image on Linux, install necessary graphics drivers:

    • On Debian-based systems (Ubuntu/Debian/Mint):

    ```
    sudo apt-get install libxss1 libglu1-mesa freeglut3
    ```

    • On RPM-based systems (CentOS/RHEL/Fedora/SUSE):

    ```
    sudo yum install libXScrnSaver mesa-libGLU freeglut
    ```
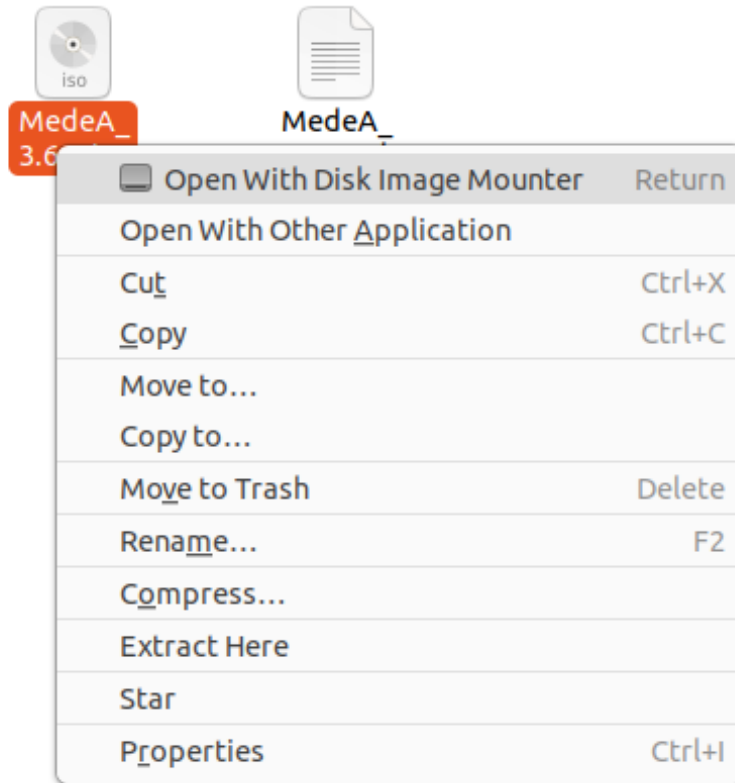
2. Use an existing directory or create a directory for the mounted drive, e.g.:

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

3. Mount the ISO image as a loop device:

    ```
    sudo mount -o loop MedeA_3.6.0.iso  /media/medea
    ```

    • Alternatively, you can also use the Disk Image Mounter tool in Linux OS (e.g. Ubuntu) to mount the ISO image.

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4. Move to the mounted drive and inside the `Linux-x64_64` directory 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.
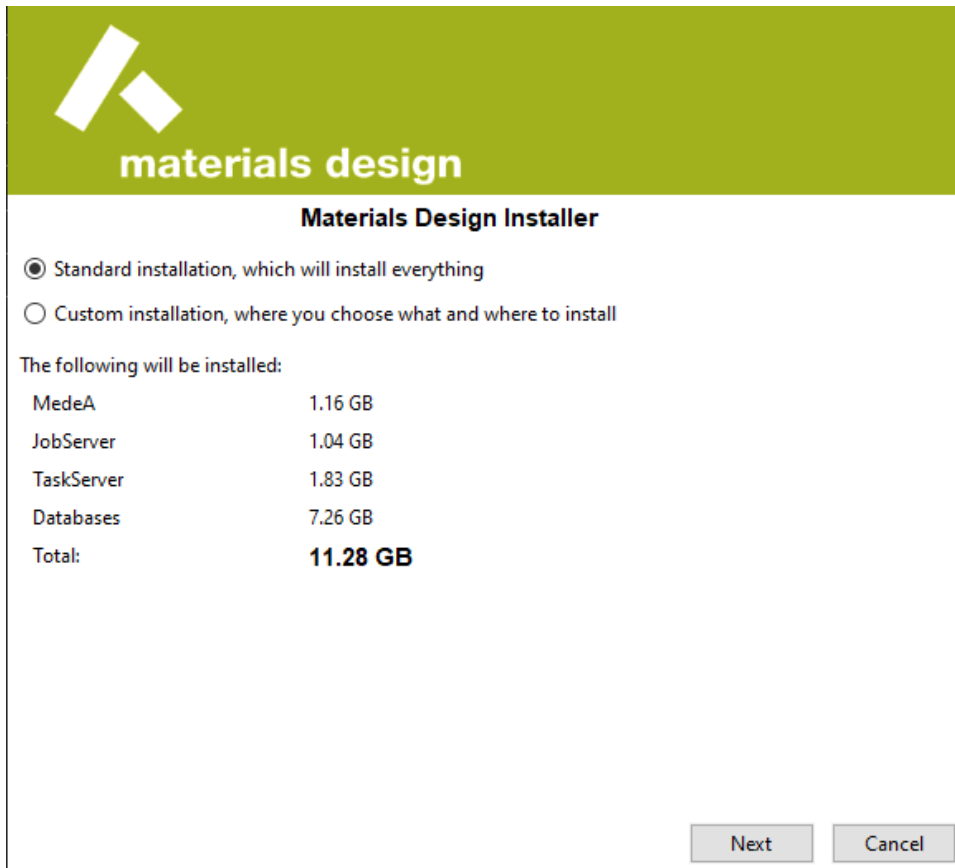
## 2.3 Installation Process

1. The *Materials Design Software Manager* window appears. Choose the option **Install MedeA Software** and click  Start :
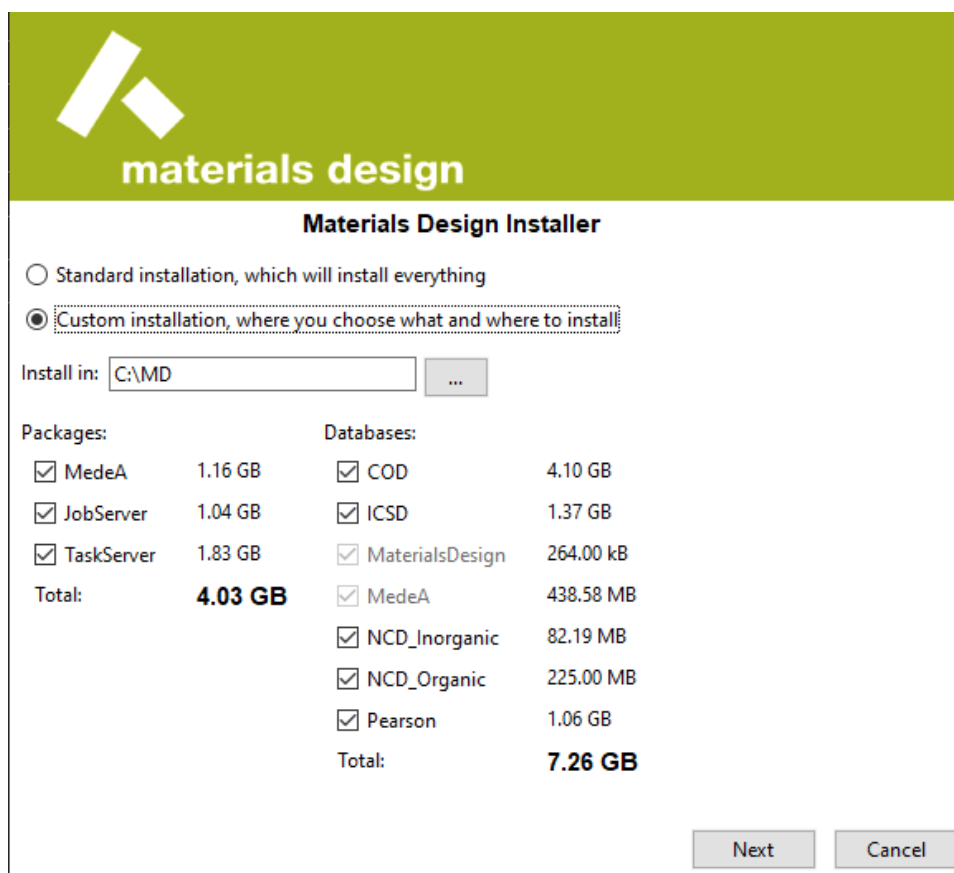
2. You have the option to choose from:

- **Standard installation**, which will install everything:



- **Custom Installation**, with which you can choose what and where to install:
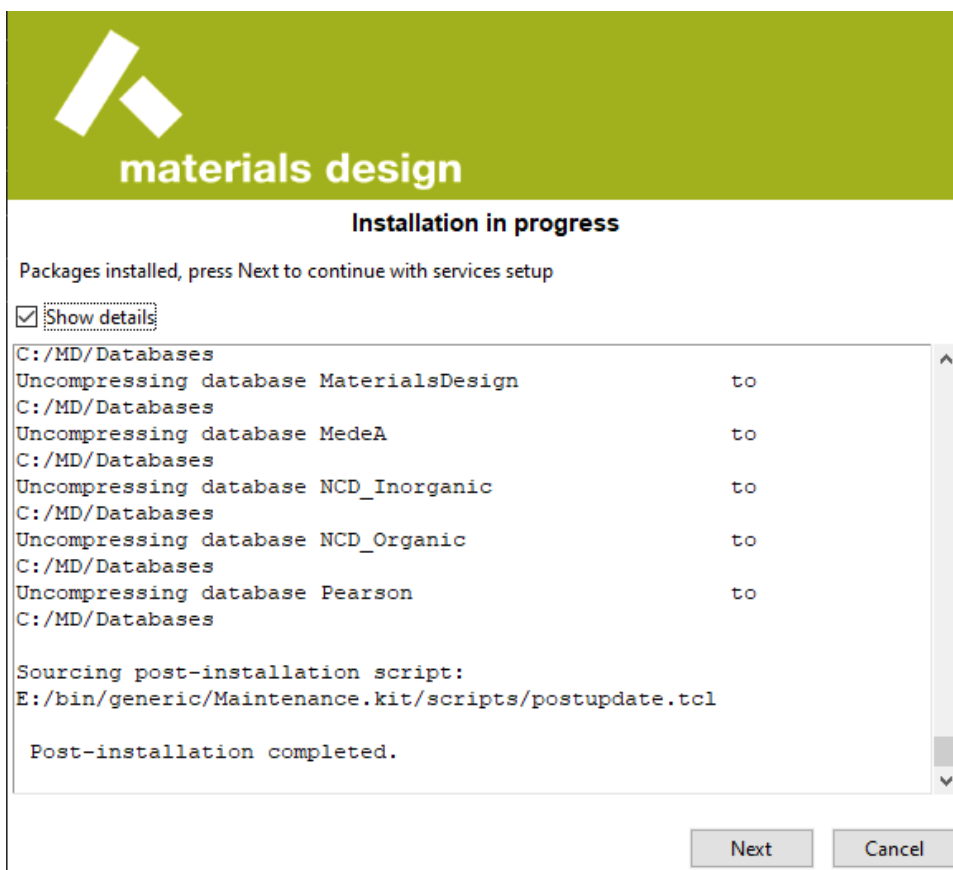
**Note:** The drive or partition you select for *MedeA* should have at least 20 GB available for storing results of calculations performed with *MedeA*.

**Warning:** On Windows, you cannot install on a user drive, which is unmounted after logging out.
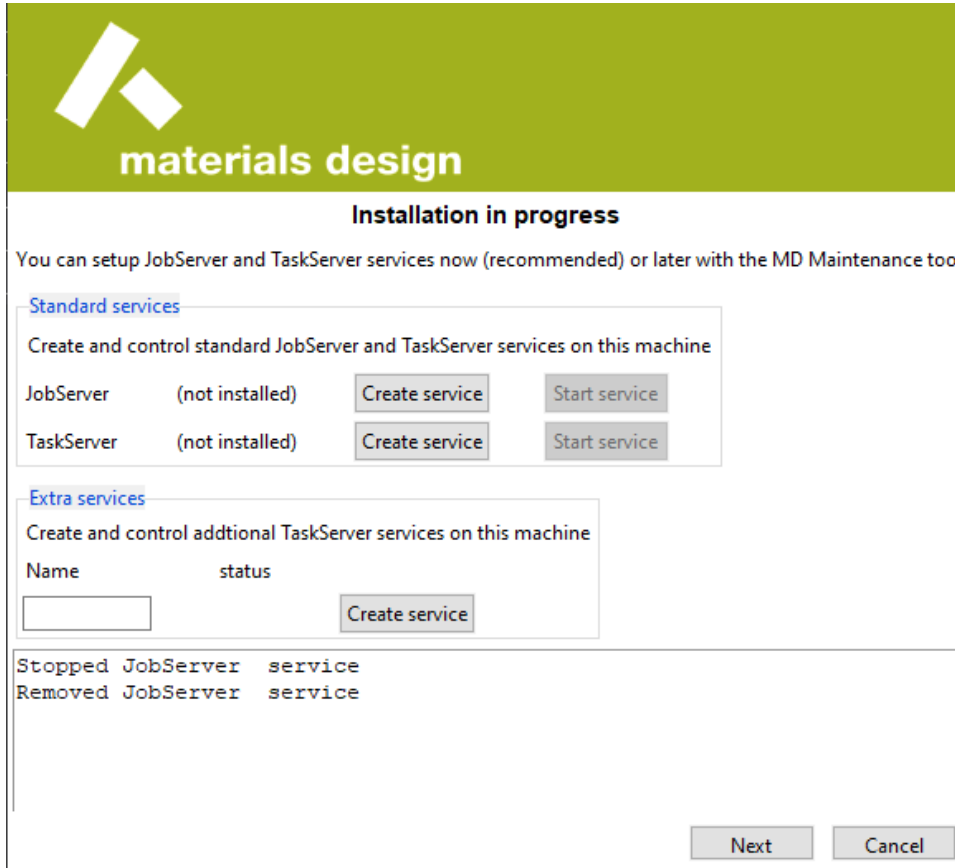
3. Make a choice and click  Next , and the installation begins:

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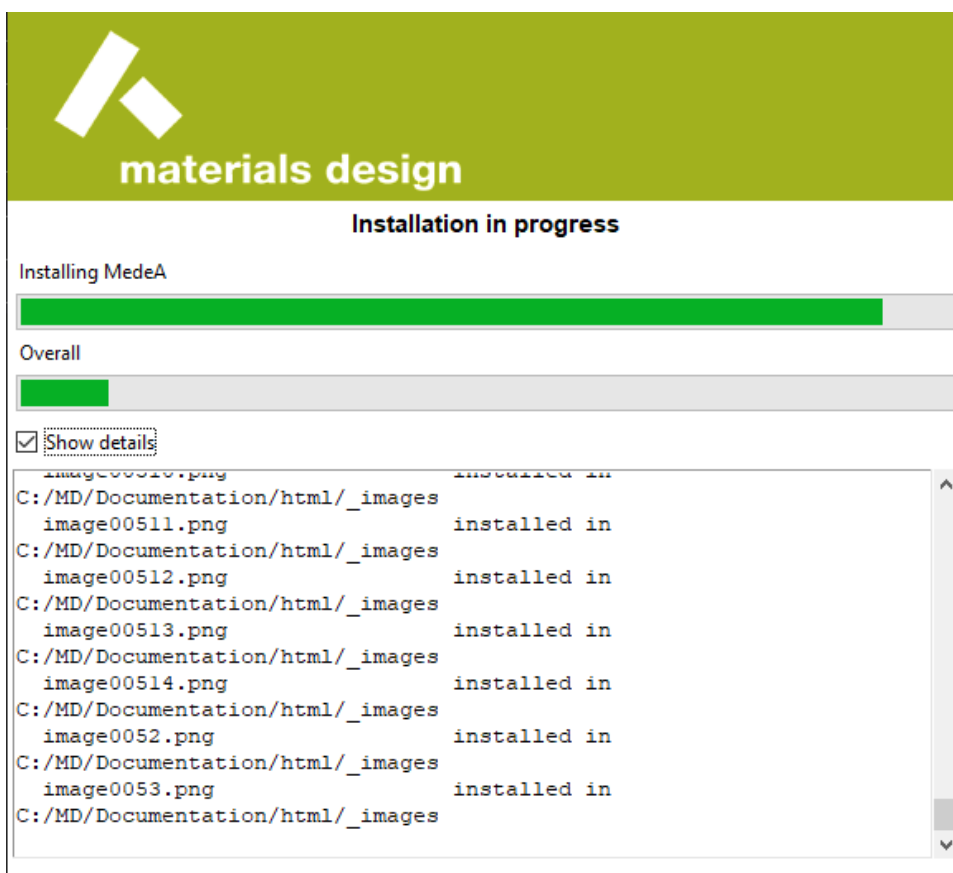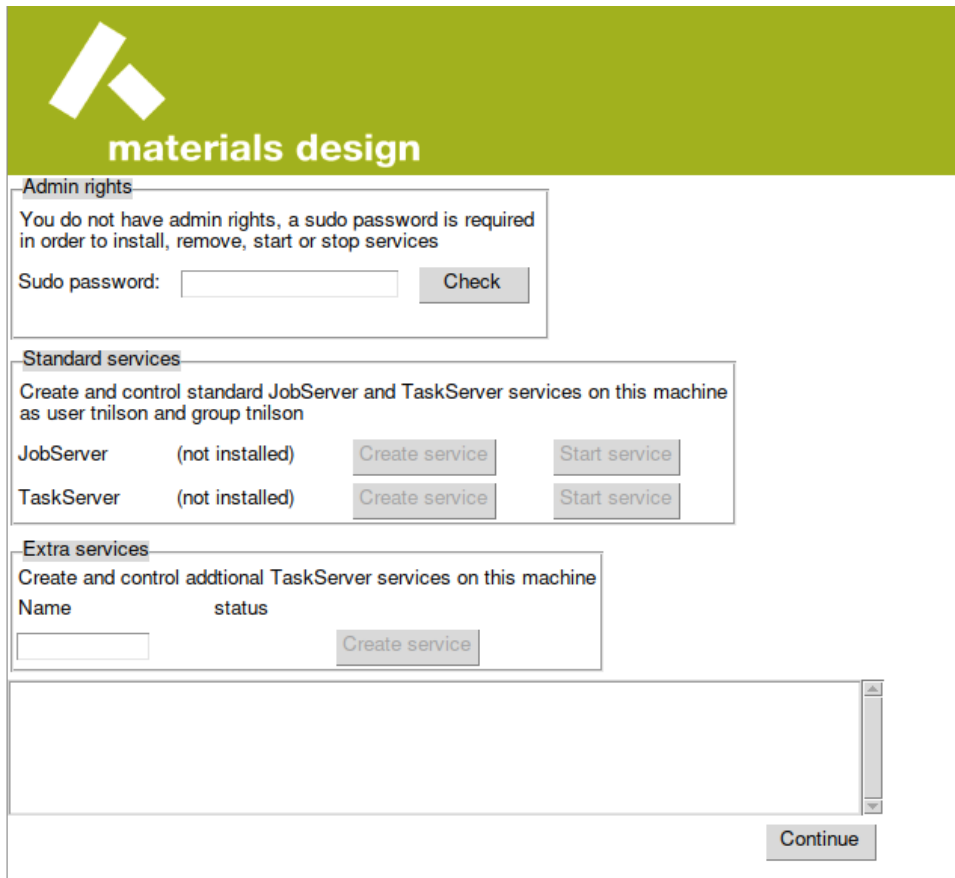
4. Click  Next  to finish the installation of the GUI:



5. The installation of JobServer and TaskServer as services follow:

On Linux, since MDMaintenance was not started with administrator rights, an option to enter your sudo password appears:
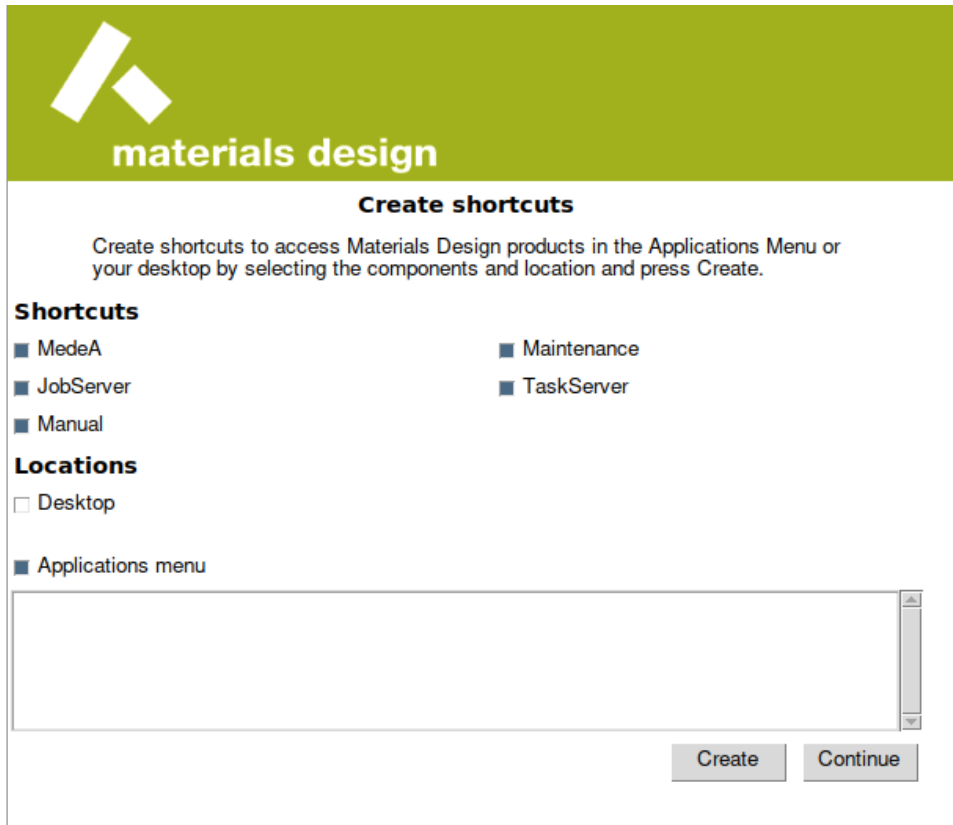
Enter your sudo password and click the `Check` button and the `Create service` buttons are enabled.

Click the `Create service` buttons then the `Start service` buttons for the JobServer and the TaskServer to install JobServer and TaskServer as services running in the background
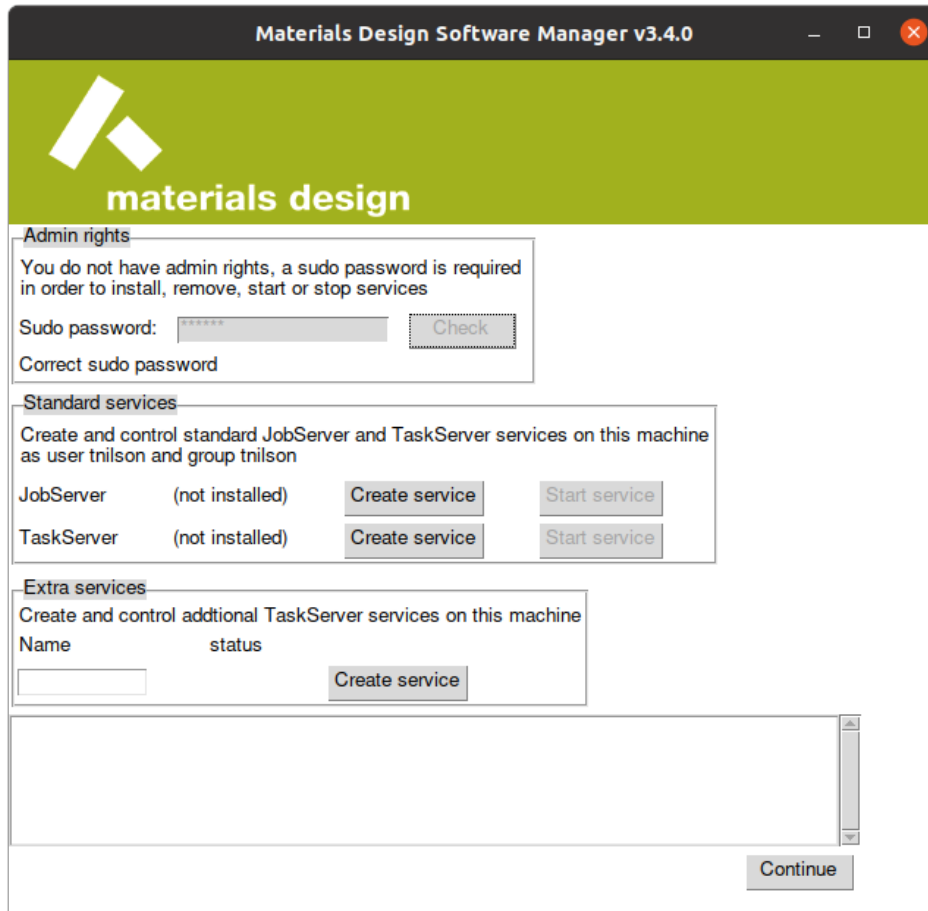


6. The next step in the installation process is to create shortcuts:
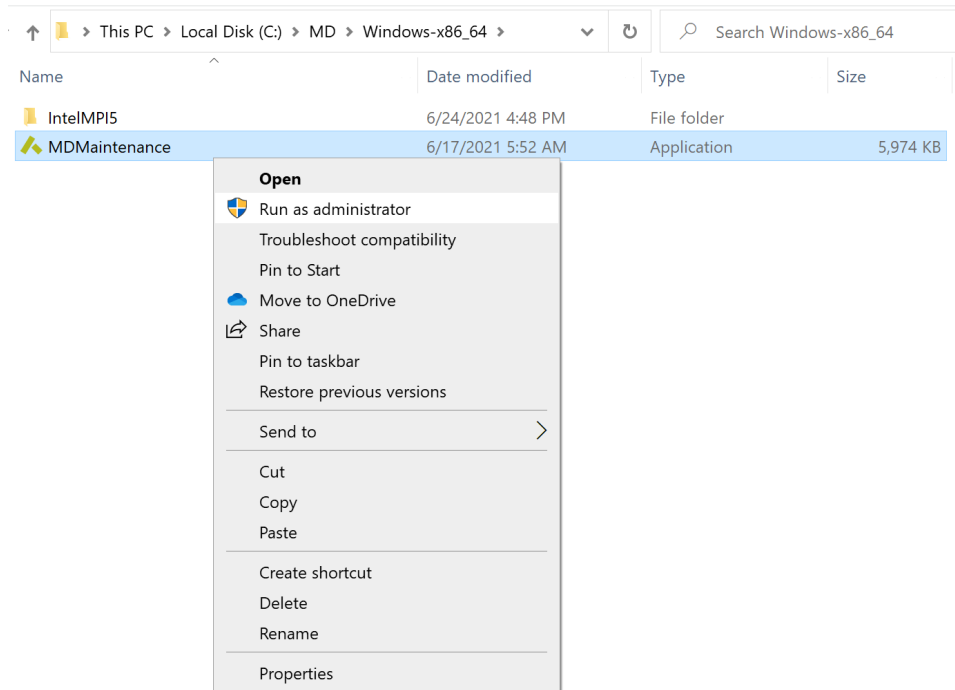
7. The installation is complete:

## 2.4 Creating Shortcuts

If by any chance no shortcuts were created on the Desktop or in the *Windows Start Menu*, you can follow these steps to create them at any time after the actual installation.

- Windows:

  Go to the *MedeA* installation directory, e.g., `C:\MD\Windows-x86_64`, right-click on `MDMaintenance` and select **Run as administrator**:

- Linux:

  Go to the *MedeA* installation directory, e.g., `/home/[username]/MD/Linux-x86_64` and start MDMaintenance:

  ```
  ./MDMaintenance
  ```

1. Click the option **Install in Applications Menu** and click  Start :



2. Make preferred selections and click  Create :
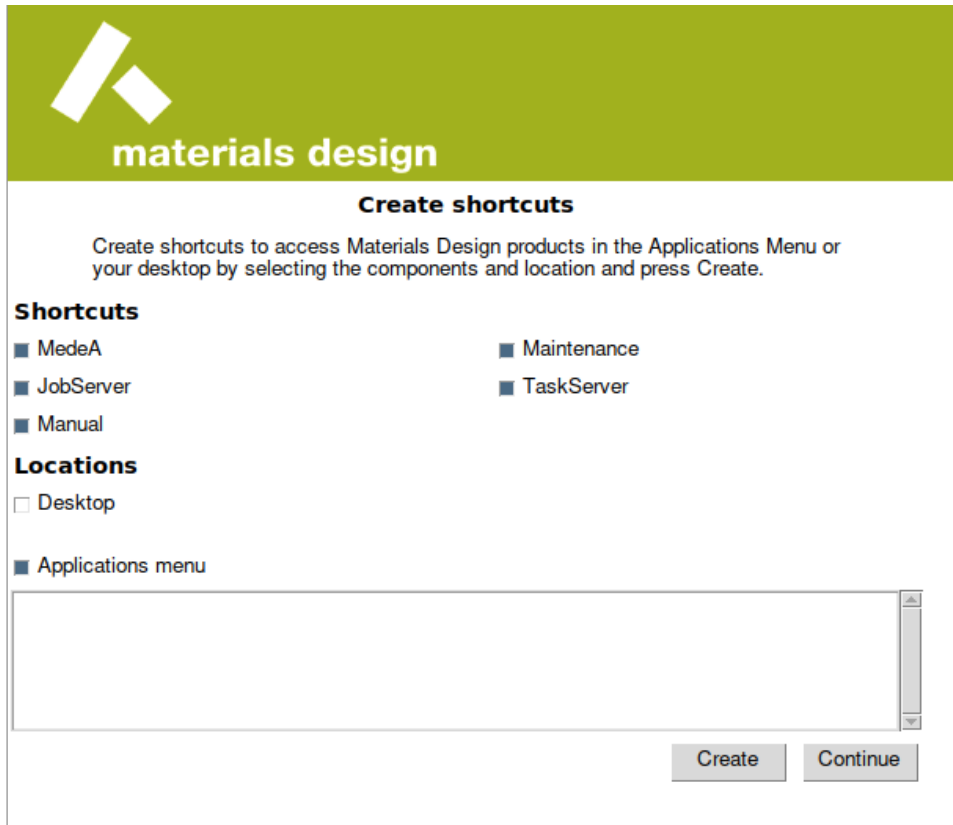
3. The shortcuts are installed on the Desktop and in the Applications menu

Use any of the shortcuts to start *MedeA* and send the license parameters as plain text to sup-port@materialsdesign.com:

# 3 Command-line Installation on Linux

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

## 3.1 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_3.6.0.iso  /media/medea
```

## 3.2 Updating *MedeA* on the Command-Line

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

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

./MDMaintenance.x -install
```

---

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

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2. Choose the installation directory:

```
=== Starting Materials Design products installation ===

Perform standard installation in folder (yes):   /home/medea/MD
or custom installation (no)
yes / no [yes]:
```

Enter `yes` to install in the default directory and `no` to a custom directory.

3. Hit `return` and follow the prompt:

```
Install MedeA (425.344 MB)?
yes / no [yes]:

Install Databases?
yes / no [yes]: no

Install JobServer (334.655 MB)?
yes / no [yes]: yes

Install TaskServer (2694.75 MB)?
yes / no [yes]: yes
```

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**Hint:** The JobServer and TaskServer do not need structure databases (neither COD, ICSD, NCD, nor Pearson)

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4. Install JobServer and TaskServer as services:

---

```
=== JobServer and TaskServer services ===

You can install JobServer and TaskServer services now or later on from the MD↵
↪Maintenance tool
Install service(s) now?
yes / no [yes]:
```

5. Enter the *sudo* password to install the JobServer and TaskServer:

```
=== Starting Materials Design services control ===

You need a sudo password to control MD services.
Password:
```

6. Choose if you would like to quit the services manager or create an extra TaskServer:

```
You can do the following:
   0 Quit services manager
   1 Stop TaskServer service
   2 Stop JobServer service
   3 Create an extra TaskServer
```

7. Decide whether to install shortcuts or not and where to install them if your choice is *yes*

```
You can do the following:
    0: proceed with selected shortcuts
    1: quit without changes
    2: unselect install to Applications menu
    3: select install to Desktop
    4: unselect shortcut MedeA
    5: unselect shortcut Maintenance
    6: unselect shortcut JobServer
    7: unselect shortcut TaskServer
    8: unselect shortcut Manual
```

8. Finish installation

9. If you have chosen to create the JobServer and TaskServer, then move to the directory, e.g. `~/MD/Linux-x86_64` and enter:

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

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

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**Note:** If you need to install JobServer and TaskServer on a shared file system on HPCs, you can execute the above commands with `sudo` or as `root` to install JobServer and TaskServer on a shared location, but ensure to change the ownership of the installed `MD` directory to the standard user (e.g. **medea** or the user's username).

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