

Installation from ISO

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1 Mounting the ISO File

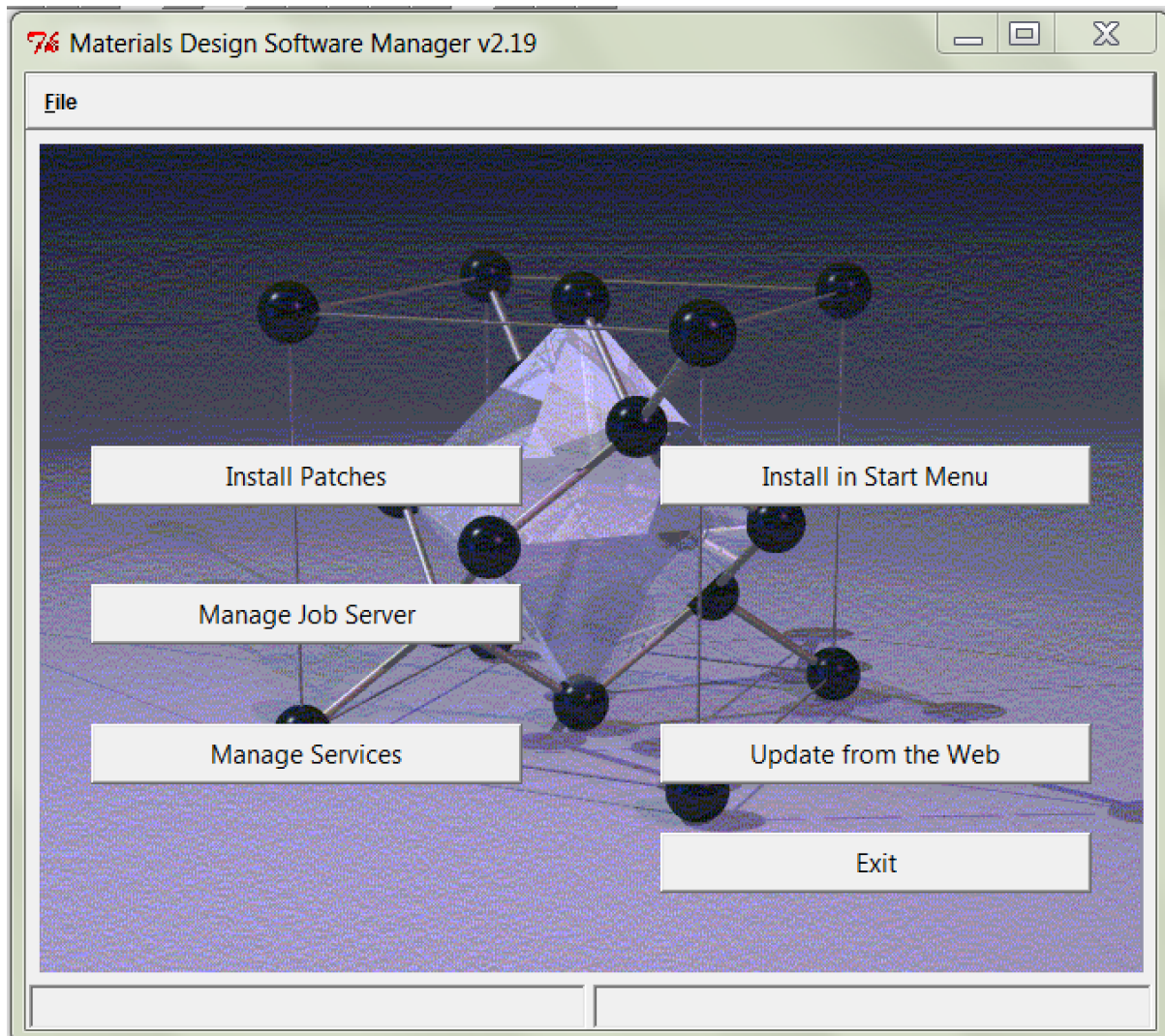
If the provided ISO only contains the ISO file `MedeA_2.22.6.iso`. You will need to mount the ISO file onto your computer to access the installer.

To do this on Windows 8 or Windows 10 right-click on the ISO file and select *Mount*. On Linux run

```
sudo mount -o loop ISO_file ~/Downloads/
```

to mount the *ISO_file* (`MedeA_2.22.6.iso`) into your *Downloads* folder. Once the ISO file is mounted you can navigate the appropriate folder, `Linux-x86_64` or `Windows-x86_64` and run the MDMaintenance program as an administrator to access the installer.

2 Installing *MedeA*

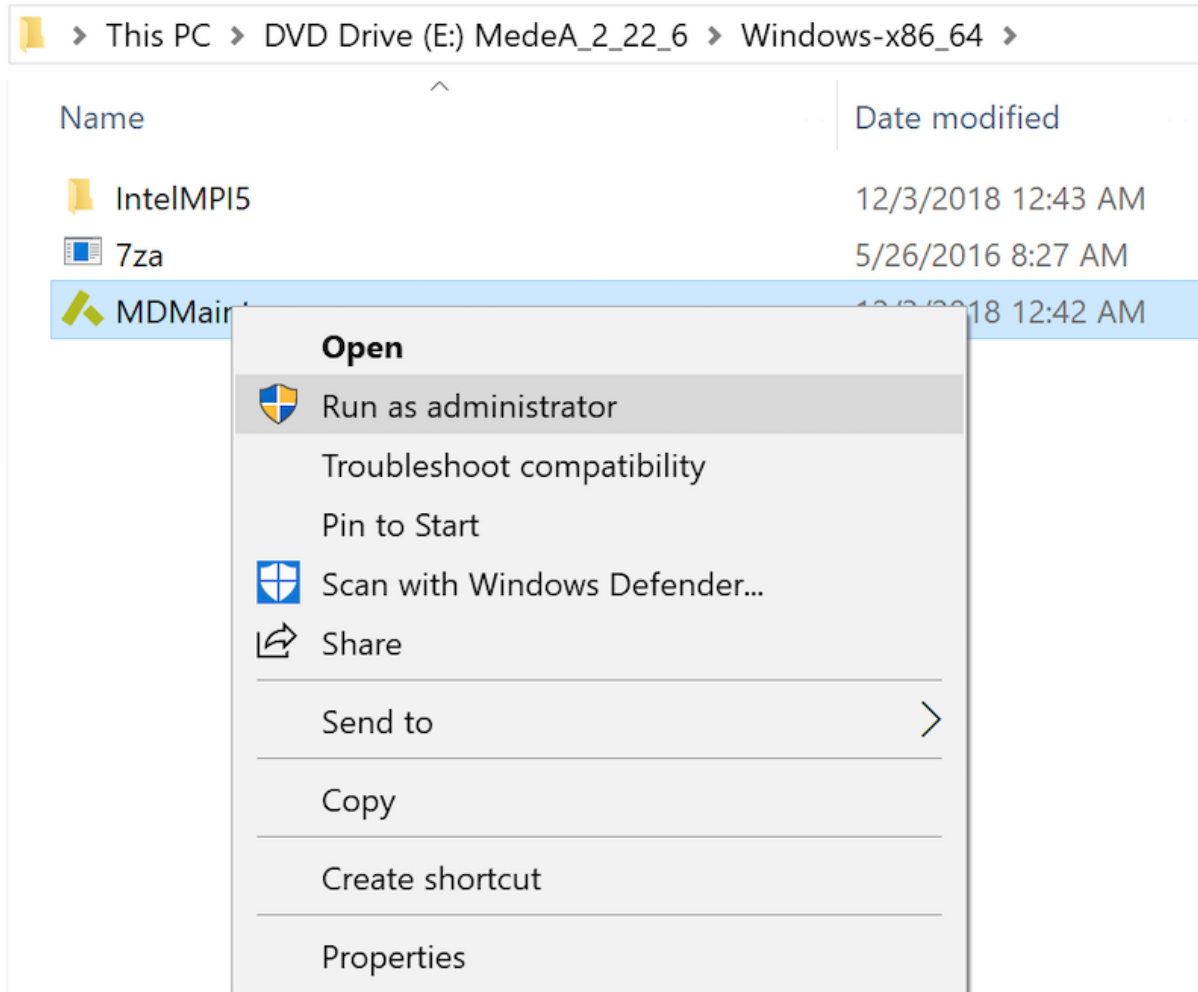


The *MedeA* installer will guide you through the installation process which will take some minutes. You will see progress updates and warnings if your system needs some changes to run some of the provided codes. At any time, you can scroll back and forth within the installer message window to inspect the individual steps of the installation.

Hint: Windows: Start the Installer as Actual User

Insert the *MedeA* ISO (or mount the ISO file) to auto start the *MedeA* Software manager. In case the Software manager does not start automatically, go to the mounted ISO drive, then into the *Windows-x86_64* directory to locate *MDMaintenance.exe*.

Right-click and select “Run as administrator”.



Hint: Linux: Start the Installer as Administrator

Create a user *medea*.

Log on as user *medea* and create the installation directory `mkdir ~/MD`

You might need to install *libXScrnSaver*, *net-tools* or similar packages missing from your distribution¹.

Run `Linux-x86_64/MDMaintenance.x` from the top level of the ISO and select `/home/medea/MD` as the installation directory.

Hint: Alternative on Linux: Start the Installer as Actual User (with *sudo* Rights)

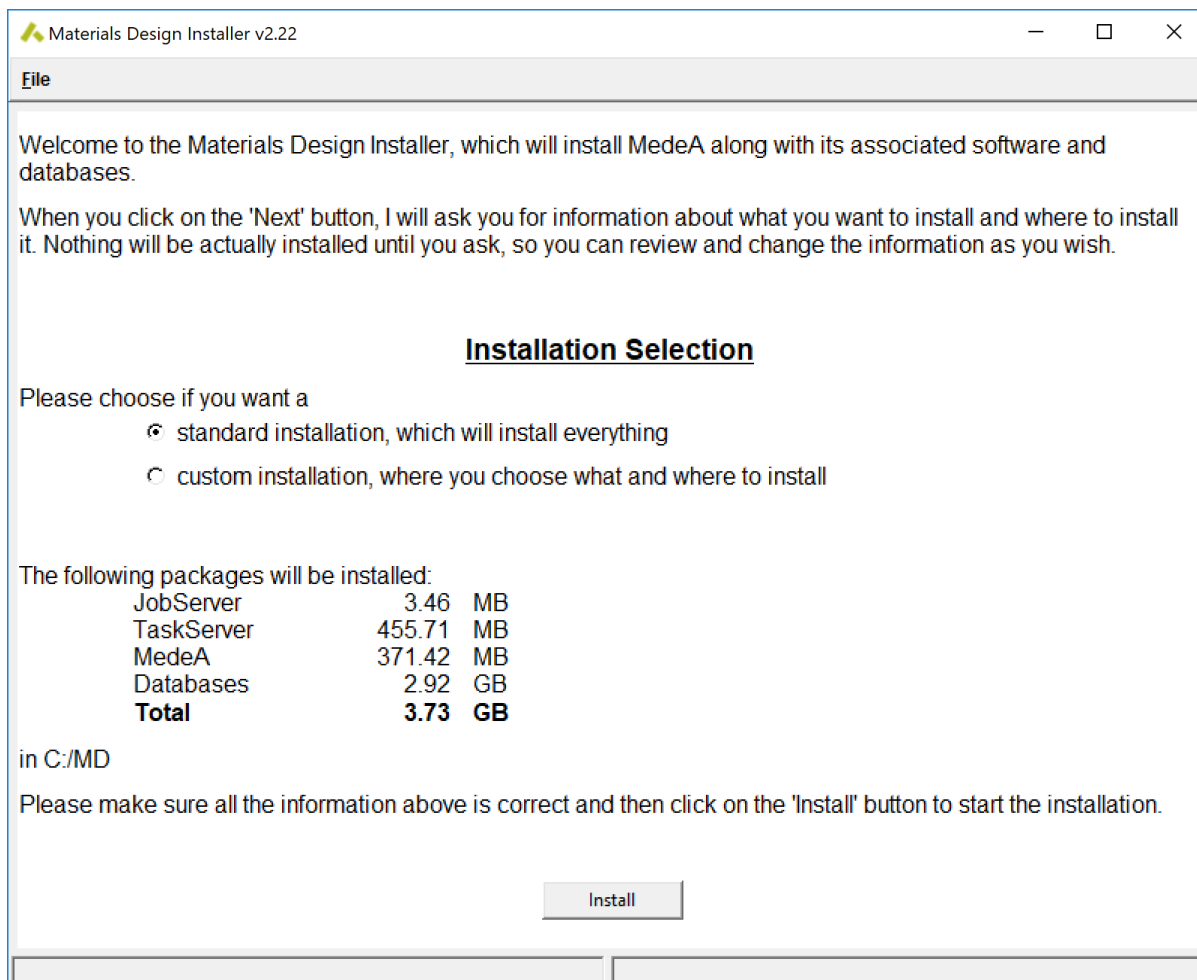
(As administrator) Create a user *medea* and give this user *sudo* rights.

Log on as user *medea* and perform the installation:

Run `Linux-x86_64/MDMaintenance.x` from the top level of the ISO

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.

Once you have *MDMaintenance* running click **Install MedeA Software** to continue and select the installation mode **standard installation** or **custom installation**. Please note that the actual size of packages and databases changes with each update and depending on the specific databases present on the ISO.



3 Standard Installation

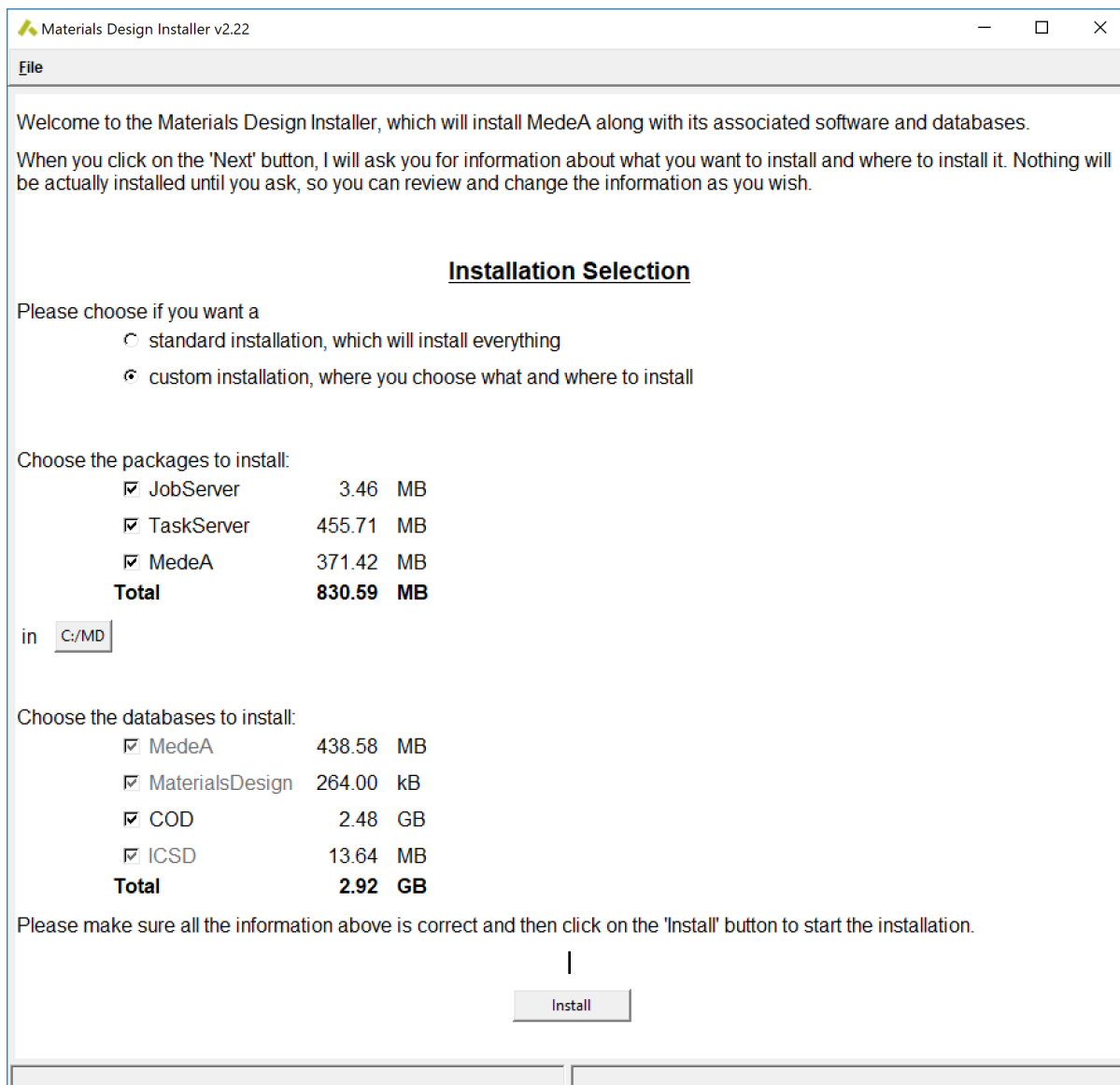
The standard installation provides default paths and installs all components from the present ISO. Note that **Standard Installation** will select *C:MD* on Windows or *~/MD* on Linux.

The drive or partition you select for *MedeA* should have at least 20 GB available for storing results of calculations performed with *MedeA*.

Hint: On Windows, you cannot install on a user drive, which is unmounted after logging out.

4 Custom Installation

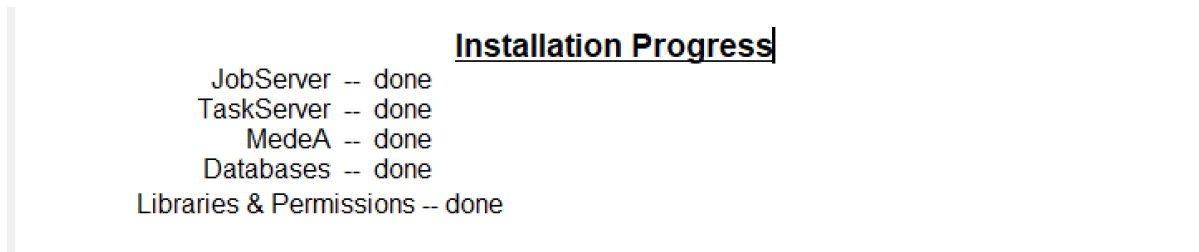
If you would like to change the *MedeA* installation or select specific modules for installation, select **Custom Installation**. Keep in mind that for maintenance it is best to have the whole *MedeA* program tree, database files, and Job data on a single hard disk partition.



- Click **Install** to continue

5 Installation Progress

In the next step, the *MedeA* installer will install all the selected *MedeA* components:



Make sure you scroll down to the very bottom of the installer window to see the latest messages. If you activate other windows while installing, the installer window may turn blank for some time before displaying an updated status. Once all components are selected, the *Installation Progress* in the installer window displays the current status, followed by done for the successful installation of each component.

6 Creating Links and Shortcuts

Install to Start Menu

Use the following dialog to put shortcuts in the Start Menu so that you can start MedeA and access JobServer and TaskServer.

Shortcuts:

MedeA JobServer TaskServer Maintenance Manual

Location:

Desktop
 Start Menu (Materials Design 2)

Create

Hint: On Linux you might see a request for your sudo password unless you install as administrator: Your password will not be shown (it appears as *****). Click on the **Check** button and it turns into an inactive **OK** button if the password is correct and you have *sudo* rights. Otherwise, you cannot install shortcuts for all users.

In this step, the installer will create shortcuts and Start menu entries for *MedeA*. Please make sure to create the start menu entries (default), as this will later be used to configure and update *MedeA*.

- Click **Create** for and you proceed to the next section.

7 Setting up JobServer and TaskServer as Services

In the next installation step, you will be asked if you would like to configure the JobServer and TaskServer as system services to start automatically during the boot phase. In order to run calculations or look at results from calculation in your browser, you need to start these processes.

We strongly recommend that you install and run these processes as system services. You can also run them as scripts, via **Start menu >> All Programs >> Materials Design 2 >> debugJobServer / debugTaskServer** on Windows. On Linux these two programs are located in *MD/2.0/JobServer/debugJobServer* and *MD/2.0/TaskServer/debugTaskServer*.

8 Verify Automatic Start of Services on Linux

Use your Linux distributions' administration tools to verify that JobServer and TaskServer will start automatically after reboot.

Check that Mdjobserver (if Installed) Starts Automatically

On *RedHat* systems the following commands are important:

```
chkconfig --list mdjobserver
```

```
mdjobserver 0:off 1:off 2:off 3:off 4:off 5:off 6:off
```

In this case, the mdjobserver is not going to start automatically. Let's change this for run levels 3 and 5:

```
chkconfig --level 35 mdjobserver on
```

```
chkconfig --list mdjobserver
```

```
mdjobserver 0:off 1:off 2:off 3:on 4:off 5:on 6:off
```

Check that mdtaskserver (If Installed) Starts Automatically

```
chkconfig --list mdtaskserver
```

```
mdtaskserver 0:off 1:off 2:off 3:off 4:off 5:off 6:off
```

In this case the mdtaskserver is not going to start automatically, change this for runlevels 3 and 5:

```
chkconfig --level 35 mdtaskserver on
```

```
chkconfig --list mdtaskserver
```

```
mdtaskserver 0:off 1:off 2:off 3:on 4:off 5:on 6:off
```

On *SuSE* use the runlevel editor of YaST. With *Debian*, *Ubuntu*, and *Gentoo* the installation of system services is part of installing mysqld.

9 Check Firewall Settings and Allow Connections for JobServer and TaskServer

If you have a firewall in place, make sure that the TaskServer can be reached from the JobServer. With *iptables* in place, the port can be opened with the following commands.

```
iptables -I INPUT -p tcp --dport 23000 -j ACCEPT
```

You can restrict access to the TaskServer to a single JobServer by specifying a network address:

```
iptables -I INPUT -p tcp --dport 23000 -j ACCEPT -s <IP of JobServer>
```

Check the current set of rules in place - and please talk to your IT department:

```
iptables --list
```

Chain INPUT (policy ACCEPT)

target prot opt source destination

ACCEPT tcp – anywhere anywhere tcp dpt:23000

To keep the set of rules working after the next reboot, you need to save them. This depends on Linux version and specifics of your installation like *RedHat/Centos/Fedora*.

```
/etc/init.d/iptables save
```

Similarly, you need to allow access on the JobServer from your GUI:

```
iptables -I INPUT -p tcp --dport 32000 -j ACCEPT
```

10 Check System Limits

Depending on model size and type of calculation, VASP and LAMMPS calculations can demand considerable amounts of memory, especially when running in parallel across many compute nodes. Please check whether the following properties are large enough, you can use *ulimit -a* in bash:

- *fsize*: maximum file size: should be *unlimited*
- *memlock*: maximum locked-in memory: 80-90% of total main memory
- *rss*: maximum memory size: should be *unlimited*
- *nofile*: number of open files: at least 20 per core
- *stack*: (memory) stack size: 80-90% of total main memory
- *cpu*: cpu time that can be used: should be *unlimited*
- *nproc*: max. processed per user: set to at least 1000
- *as*: virtual memory: should be *unlimited*
- *Locks*: file locks: should be *unlimited*

Modify `/etc/security/limits.conf` to raise the impinging limits, here are examples:

End of file

* soft memlock unlimited

* hard memlock unlimited

* soft nofile 10240

* hard nofile 10240

* soft nproc 3153919

* hard nproc 3153919

Hint: You can replace * with *medea* to limit those changes to the TaskServer running as user *medea*. Remember to restart the TaskServer to use the changed limits.

11 Installing TaskServer/s on Multiple Machines

For configurations with multiple TaskServer/s you have to repeat the TaskServer/s installation on each machine:

- Perform a **Custom Installation** in case you want to change the installation path; otherwise the **Default Installation**.

You can keep your *MedeA* installation up to date using the installed maintenance program (MDMaintenance) to update from the web. This will download the current version of modules and codes.