

Requirements and Installation Scenarios

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1 Introduction

This section describes the hardware and software requirements for installing and running *MedeA*. The tiered architecture of *MedeA* lets you combine components in several ways thus adapting to the needs of your specific compute environment. This section also describes the different installation scenarios.

Warning: *MedeA* does not support 32-bit operating systems anymore. Please upgrade your operating systems to 64-bit systems before installing *MedeA*.

2 Requirements

2.1 Computer Specifications

Component	Requirement
Operating system (oldest supported versions listed; newer versions also supported)	Windows: 10; Linux: RHEL 7, CentOS 7.9, Fedora 19, SUSE 12.5, Oracle 7.9, Debian 10, Ubuntu 20.04, Mint 20
Architecture/Processor	All x86-64 bit architectures from Intel and AMD: Opteron, Ryzen, Zen, Core2, Core2Duo, i5, i7, i9, Xeon. ARM and Power8 are not supported.
CPU speed	Strong floating-point performance required. No lower/upper hard limit on clock speed
GPU	For best double-precision performance, Nvidia Tesla series (Kepler, Pascal, Volta, and Turing) are strongly recommended. For workstations and desktops, GeForce Titan V, Quadro GV100, and Quadro GP100 are recommended.
Memory	1–4 GB RAM per core; 4 GB/core is recommended for VASP
Disk space	6 GB minimum for a full <i>MedeA</i> installation, no lower/upper hard limit for storing user generated data
Graphics	Support of OpenGL 2.1 and higher and at least 128 MB of memory
Network	Fast Ethernet, 100 Mbps or faster if GUI/JS/TS are on different machines. No network access required if all three tiers are on the same machine.
Display	Screen resolution of 1280x800 at minimum, recommended 1920x1080

2.2 Software

MedeA will install on Windows without additional software. However, on some Linux installations, additional packages need to be installed.

Debian-based systems

On Debian-based systems such as Debian, Ubuntu, and Mint please install these packages using *apt install*.

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

RPM-based systems

On RPM-based systems such as CentOS/RHEL, Fedora, and OpenSUSE please install these packages using *yum install*.

```
sudo yum install libXScrnSaver mesa-libGLU freeglut
```

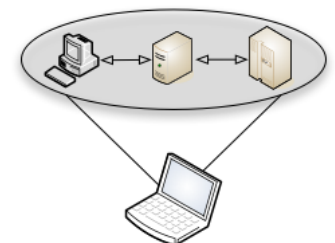
Note: On Linux, only the X11 display server is fully supported. Please avoid using the Wayland display server

3 Installation Scenarios

The tiered architecture of *MedeA* lets you combine components in many ways thus adapting to the needs of your specific compute environment. Here are a few scenarios of how to install the software:

3.1 Single Machine

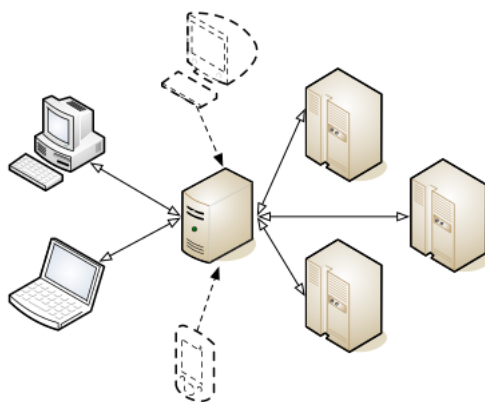
In a stand-alone configuration, *MedeA* runs on a single Windows or Linux machine having one or multiple processing units (e.g. multicore CPUs). All components, that is the graphical user interface (GUI), the structure databases, JobServer, (and job databases) and the TaskServer are installed on this machine and all computations run locally. Access the web interface of the JobServer from any smartphone or other computer.



Procedure

1. Download installation medium (Windows .exe installer or ISO image)
2. Mount installation medium
3. Perform default installation
4. Start *MedeA*
5. Request license file and copy the received license file to the root of the installation directory (top-level folder).
6. Restart *MedeA*

3.2 Small Cluster



- One or more PCs, each running the *MedeA GUI*
- A **single, central JobServer** on one of the above machines or on a dedicated machine
- **TaskServers** on some/each of the above machines; additional TaskServers on other networked resources (Windows/Linux)
- Access to the web interface of the JobServer from any smartphone or computer

There is a single, central JobServer.

Laptops can have a local JobServer to work when operating as a stand-alone single machine, but all computations on the shared TaskServer go through the central JobServer.

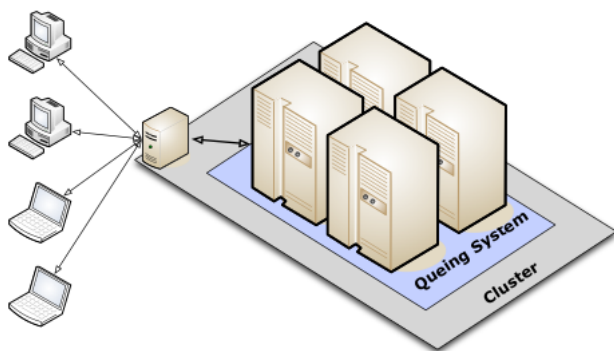
Procedure

1. Download installation medium

2. Mount installation medium to JobServer
3. Default installation on JobServer
4. TaskServers
 - (a) In case the TaskServer does not share the *MedeA* installation folder (e.g. *C:/MedeA* or *~/MD/MedeA*):
 - (b) Mount installation medium to JobServer
 - i. Custom installation TaskServer on any TaskServer
 - (c) With shared *MedeA* installation folder (e.g. */export/MedeA*):
 - i. Start Maintenance Program on TaskServer and create TaskServer daemon
5. Mount installation medium to the frontend
6. Perform default installation
7. Start *MedeA GUI* on the frontend
8. Request license file for GUI
9. Restart *MedeA GUI*

Hint: You do not need a license file for computers without *MedeA GUI* installed which are running as JobServer and TaskServers only.

3.3 Larger Clusters and External Queuing Systems



When several compute-intensive applications share the same resources, it is recommended to make use of queuing systems like e.g. *PBS*, *LSF*, *SLURM*, *GridEngine*, or *LoadLeveler*. The *MedeA* TaskServer supports external queuing systems under Linux/Unix by providing templates for queue submission (batch) scripts.

Note: *MedeA* does not provide management tools for external queuing systems. You will need to adapt the template scripts provided along with the TaskServer to fit your local installation. The current implementation requires one TaskServer client per queue type and queuing system to be installed on the gateway machine that is the login or the head node of a supercomputer or massively parallel machine. Configurable scripts for the PBS, LSF, SLURM, and GridEngine queuing systems are provided for each of the computationally intensive codes (VASP, LAMMPS, Gaussian, MOPAC, and GIBBS) in relevant subfolders of *C:\MD\TaskServer\Tools* or *~/MD/TaskServer/Tools*.

Procedure

1. Download installation medium
2. Mount installation medium to JobServer

3. Default installation on JobServer
 4. TaskServer
 - (a) In case TaskServer does not share *MedeA* installation folder (e.g. *C:/MedeA* or *~/MD/MedeA*):
 - i. Mount installation medium to JobServer
 - ii. Custom installation TaskServer on any TaskServer
 - (b) With shared *MedeA* installation folder (e.g. *C:/MedeA* or *~/MD/MedeA*):
 - i. Start Maintenance Program on TaskServer and create TaskServer daemon
 5. Configure queuing system integration
 6. Mount installation medium to frontend
 7. Perform default installation
 8. Start *MedeA GUI* on the frontend
 9. Request license file for GUI
 10. Restart *MedeA GUI*
- For more information of installing *MedeA* on a cluster see the HPC Configuration section.