Installation scenarios

Contents

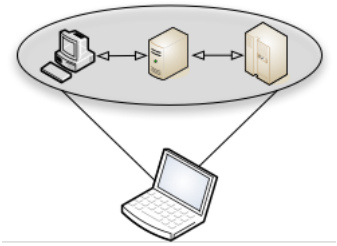
1 Installation Scenarios

1.1 Introduction

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

1.2 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, the structure databases, JobServer, (and job databases) and the TaskServer are installed on this machine and all computations run locally.

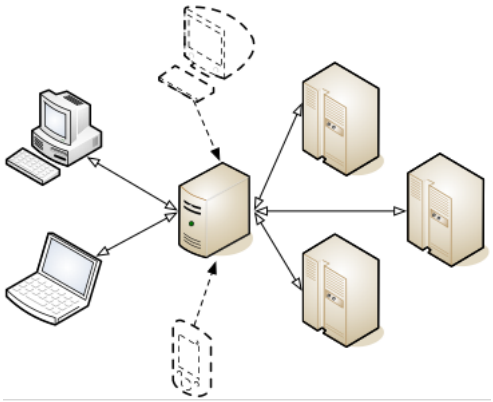


Procedure

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 MD/2.0
6. Restart *MedeA*

DOCUMENTATION

1.3 Small Cluster



- One or more PCs, each running the *MedeA GUI*
- A **single, central JobServer** on one of the above machines or a dedicated machine
- **TaskServer**s on some/each of the above machines, additional TaskServers on other networked resources (Windows/Linux)
- Access to the JobServer's web interface 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 TaskServer does not share the *MedeA* installation folder (*MD/*):
   (b) Mount Installation medium to JobServer
      i. Custom Installation TaskServer on any TaskServer
   (c) With shared *MedeA* installation folder (*MD/*):
      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 TaskServer

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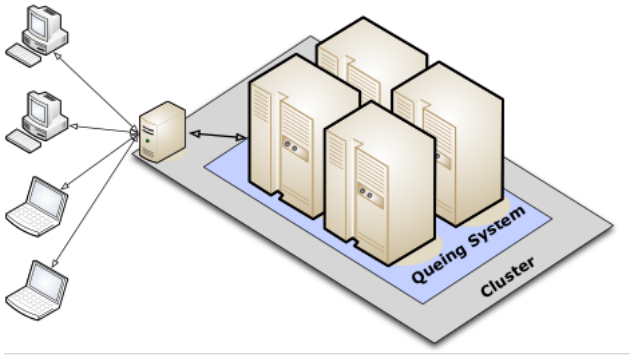
1.4 Larger Clusters and External Queuing Systems



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

Note that *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:MD2.0TaskServerTools* or *~/MD/2.0/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 (*MD/*):
      i. Mount Installation medium to JobServer
      ii. Custom Installation TaskServer on any TaskServer
   (b) With shared *MedeA* installation folder (*MD/*):
      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*