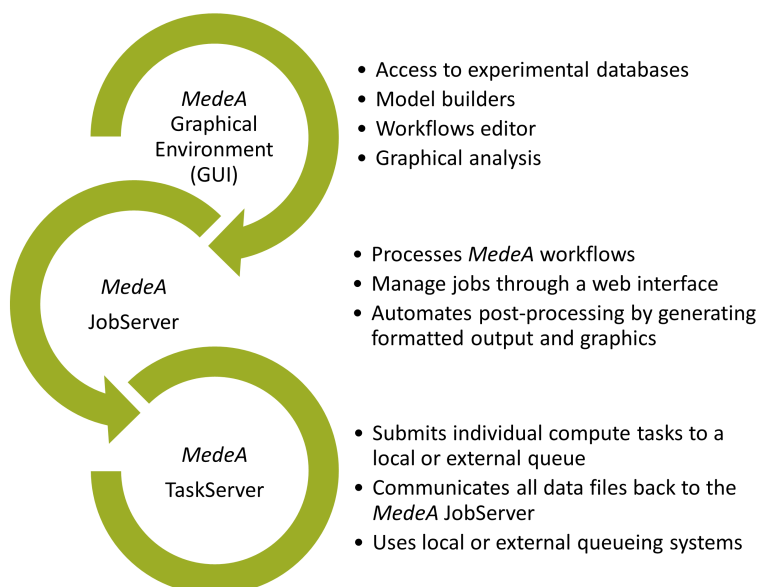**materials design®**

# Overview of MedeA Installation

The three-tiered architecture of *MedeA* consists of the *MedeA* graphical environment (GUI, main tier), the JobServer (middle tier), and the TaskServer (end tier).

The middle tier or the JobServer is the central hub for controlling computational jobs, job pre-processing, and job post-processing. The JobServer maintains a database of job-related data and stores computational results on disk. A *MedeA Job* is a workflow or protocol generated by a *MedeA* compute engine GUI or by the *MedeA* flowchart editor. A typical *Job* may generate one or multiple tasks using *MedeA* compute engines.

The end tier or the TaskServer submits individual tasks, parts of a *MedeA* Job, to the internal queuing system of *MedeA* or to an external queuing systems such as LSF, PBS, or similar schedulers. One or several TaskServers can be configured and connected to a JobServer. All communication between a TaskServer and the GUI flows through the JobServer.



*MedeA* Graphical Environment (GUI)
- Access to experimental databases
- Model builders
- Workflows editor
- Graphical analysis

*MedeA* JobServer
- Processes *MedeA* workflows
- Manage jobs through a web interface
- Automates post-processing by generating formatted output and graphics

*MedeA* TaskServer
- Submits individual compute tasks to a local or external queue
- Communicates all data files back to the *MedeA* JobServer
- Uses local or external queueing systems

The three tiers can be installed on the same or different machines; there is no conceptual difference between running the GUI, JobServer, and TaskServer on one laptop or using separate machines.



GUI         JobServer         TaskServer

A single installation ISO image allows installing the *MedeA* GUI, JobServer, and TaskServer (including the *MedeA* compute engines *VASP*, *LAMMPS*, *GIBBS*, *Gaussian*, and *MOPAC*) on either Windows or Linux operating systems. *MedeA* uses an integrated version of SQLite to manage experimental databases, code specific data, and data generated by the user.