



JobServer & TaskServer

Indispensable for High Performance Computing

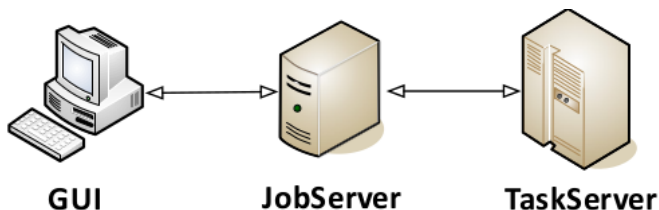
At-a-Glance

MedeA's^{®1} JobServer & TaskServer is the central unit to manage, monitor, and archive your calculations efficiently and consistently. Thanks to the MedeA's JobServer & TaskServer, a highly flexible workflow maximizes productivity, even on systems with heterogeneous hardware, and different operating systems.

Key Benefits

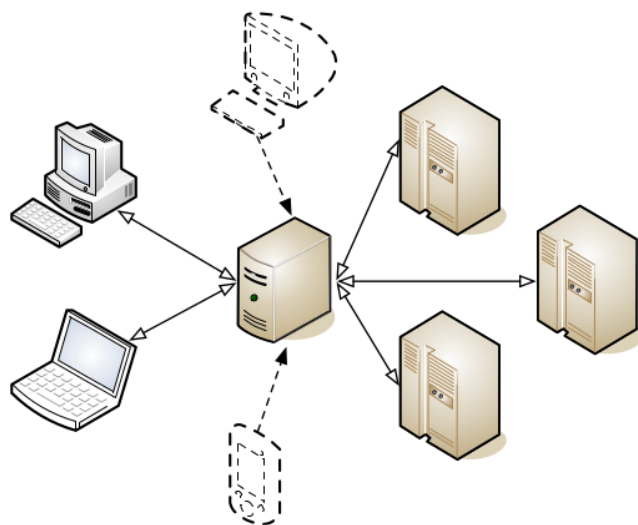
- Automated processing of compute protocols and workflows
- Machine driven post-processing and results analysis of calculations with the following compute engines: VASP, LAMMPS, GIBBS, MOPAC, and GAUSSIAN
- Robust leveraging of compute resources from small-sized clusters to high performance computing systems
- Reliable long-term archiving and accounting of computed data

MedeA has a unique three-tiered architecture: The MedeA GUI as the top tier, the JobServer as the middle tier, and the TaskServer as the bottom tier.

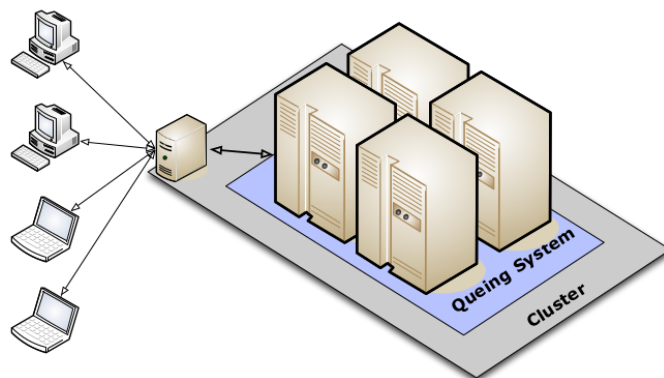


For smaller compute clusters, easily install a single central JobServer on a dedicated machine, and install TaskServers on the compute nodes. With this setup, submit calculations from one or more computers, which have the MedeA GUI's installed. MedeA's JobServer & TaskServer have web interfaces to manage and monitor jobs, and restrict access if necessary.

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Use the JobServer & TaskServer as a gateway for high performance computing in computer centers or the cloud. The JobServer & TaskServer support the most common load balancing systems such as SLURM, PBS/Torque, and GridEngine.



*'*MedeA's* JobServer and TaskServer automatically and reliably process your jobs and calculations while you are thinking about your next groundbreaking innovation in materials science.'*

Specifications

- MedeA's JobServer & TaskServer require a 64-bit Intel or AMD architectures, and can be driven by various Windows or Linux operating systems.

- Windows Server 2008/2012/2016, Windows 7/8/10
- Linux: CentOS, Redhat, Debian , Fedora , SuSE , Ubuntu , Oracle
- Memory requirements: 1-4 GB RAM per compute core
- Hard Drive space:
 - 5 GB minimum for a full *MedeA* installation
 - 60-180 GB for storing user generated data
- Supported queuing (load balancing) systems are:
 - PBS/Torque
 - SLURM
 - GridEngine
 - LSF
 - Windows HPC

- JobServer updates and maintenance are possible without interrupting running calculations
- Easy exchange of jobs and data between JobServers

Key Features

- Compute Management
 - Automated processing of compute protocols and workflows
 - Web interface designed for on-the-fly job monitoring: hold/resume, restart, etc.
 - Flexible administration of computer resources, even in heterogeneous systems
 - Developed for multi-user operation
- Results & Data Management
 - Quick job search filters for users, status, title, and date
 - Efficient and consistent accounting of jobs and relevant files
 - Job index in an SQLite database while data is stored on disk
 - Full access to all input and output files for authorized users
 - Share results and workflows with a team
- Security & Integrity
 - JobServer & TaskServer run as system services (daemons) for continuous access
 - Secure communication and access via HTTPS
 - User authentication restricts access and prohibits data vulnerability
- Maintenance

Required Modules

- *MedeA Environment*

Tightly Integrated Modules

- *MedeA Interface Builder*
- *MedeA VASP*
- *MedeA MOPAC*
- *MedeA Gaussian GUI*
- *MedeA GIBBS*
- *MedeA EAM*
- *MedeA Phonon*
- *MedeA Transition State Search*
- *MedeA MT*
- *MedeA UNCLE*
- *MedeA HT-Launchpad*
- *MedeA HT-Descriptor*
- *MedeA Forcefield Optimizer*
- *MedeA Diffusion*
- *MedeA Thermal Conductivity*
- *MedeA Viscosity*
- *MedeA CED*
- *MedeA Surface Tension*
- *MedeA Electronics*

Supported Modules

- All *MedeA* modules

Find Out More

Learn more about submitting and monitoring computations in the *MedeA Environment* from our Webinar:

- [An Introduction to the MedeA user interface](#)