JobServer & TaskServer

Indispensable for High Performance Computing

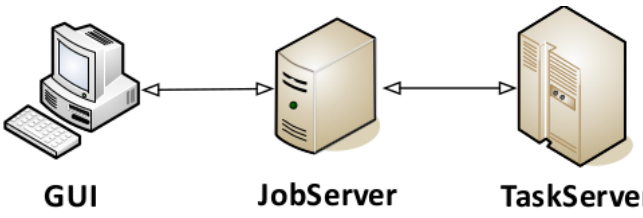
At-a-Glance

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

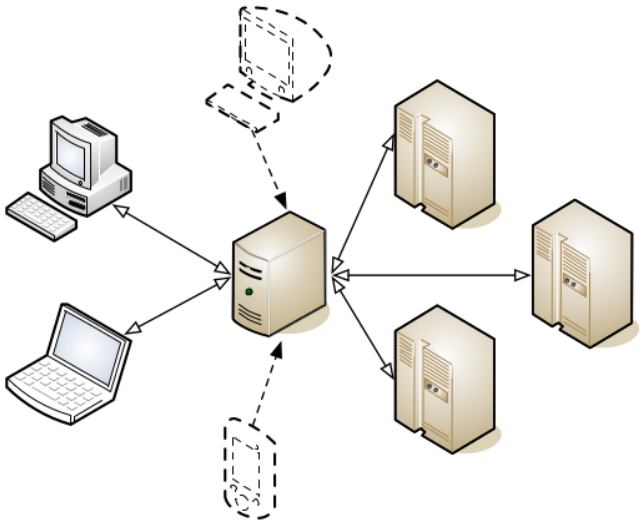
- Automated processing of compute protocols and workflows
- Machine driven post-processing and results analysis of calculations with the following compute engines: VASP, LAMMPS, GIBBS, MOPAC, and GAUSSIAN
- Robust leveraging of compute resources from small-sized clusters to high performance computing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

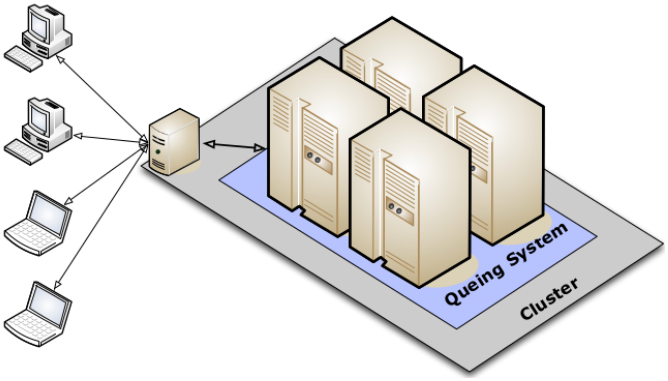


For smaller compute clusters, easily install a single central JobServer on a dedicated machine, and install TaskServers on the compute nodes. With this setup, submit calculations from one or more computers, which have the *MedeA GUI's* installed. *MedeA's* JobServer & TaskServer have web interfaces to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

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.



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 , Fedroa , 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

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

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

12121 Scripps Summit Drive, Suite 160 San Diego CA 92131, USA
P: +1 760 495-4924 - F: +1 760 897-2179 - E: info@materialsdesign.com