

JobServer and TaskServer Administration and Configuration

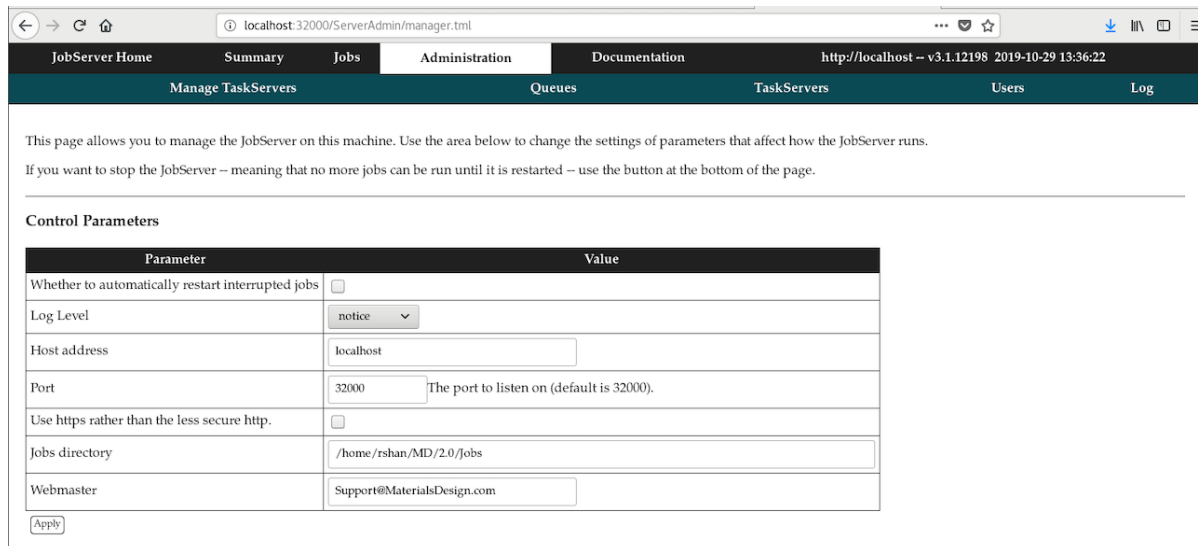
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1 JobServer Administration and Configuration

The JobServer is the middle tier of *MedeA*. It executes the jobs launched in the *MedeA* graphical user interface (the first tier). Jobs contain one or a series of tasks, created by a single job or a flowchart, that are executed by the *TaskServer*.

The JobServer can be accessed by selecting **View and Control Jobs** from the **Jobs** menu in the *MedeA* GUI. Also, the JobServer running on the computer with the GUI installed can be accessed from <http://localhost:32000> [1]. The JobServer page is primarily used for monitoring jobs. Please see the Monitoring a Running Job section for more information. Once on the JobServer page click the **Administration** tab to change the settings of the JobServer.



This page allows you to manage the JobServer on this machine. Use the area below to change the settings of parameters that affect how the JobServer runs. If you want to stop the JobServer – meaning that no more jobs can be run until it is restarted – use the button at the bottom of the page.

Control Parameters

Parameter	Value
Whether to automatically restart interrupted jobs	<input type="checkbox"/>
Log Level	notice
Host address	localhost
Port	32000 <small>The port to listen on (default is 32000).</small>
Use https rather than the less secure http.	<input type="checkbox"/>
Jobs directory	/home/rshan/MD/2.0/jobs
Webmaster	Support@MaterialsDesign.com

Apply

On this page you can set the **Log Level**. The default level is *notice*; however, this can be changed to *debug* if you are having issues configuring the JobServer. The **Host address** is name of the JobServer and we recommend changing it to *localhost*. The **Port** is the port number that the JobServer is running on.

The **Jobs directory** is directory where all the job files are stored according to their job id number. The default directory of the JobServer is *MD/2.0/Jobs*. All the input and output files will be stored here after all the tasks have finished, see the next section *TaskServer* to administrate tasks.

[1] <http://localhost:32000/>

Warning: The port for the JobServer needs to be open in you firewall settings.

The configuration file (*JobSever.options*) for the JobServer is located in in the *MD/2.0/JobServer* directory. You can make changes to this file that will directly change the JobServer settings and appear on the JobServer page.

Warning: Incorrect settings in the *JobSever.options* will cause the JobServer to produce an error upon start and not run.

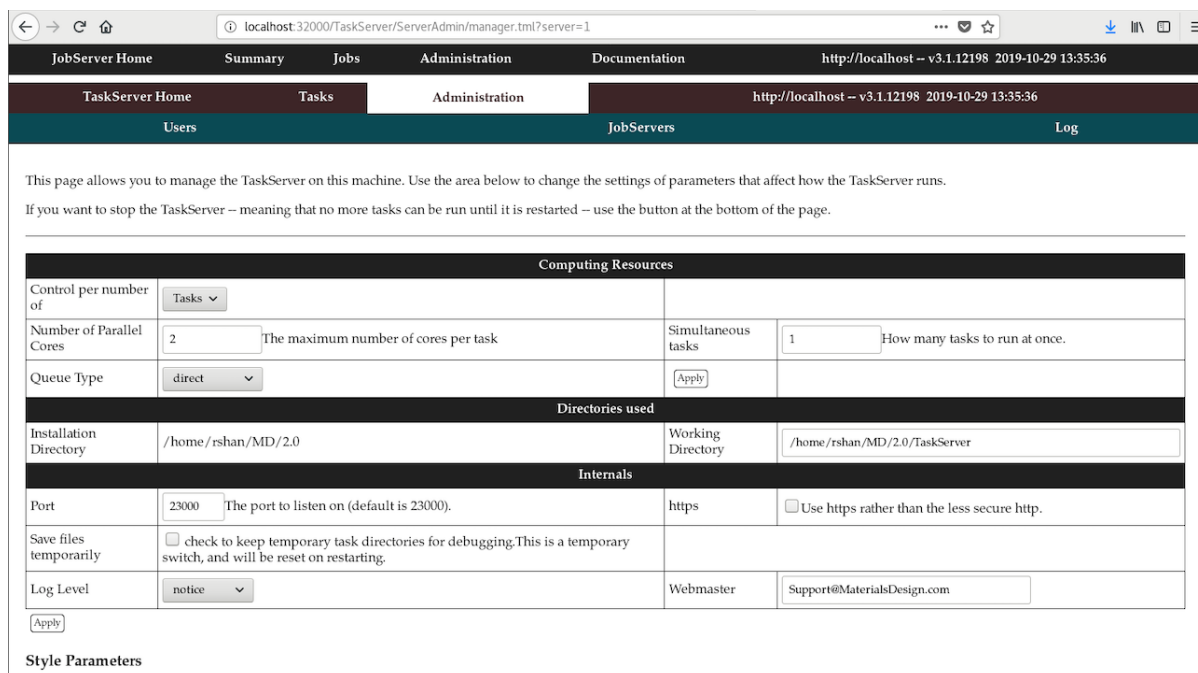
MedeA stores job information in its *MDJobs.db* database and in the *MD/Databases* directory. This database contains all the information displayed on the Jobs page. Jobs can be added to this database using the **Import/Reconnect Jobs** function in **Import/Reconnect Jobs** in the Materials Design Maintenance program, see the Using the Materials Design Maintenance Program section for more information.

2 TaskServer Administration

The TaskServer is the end tier of *MedeA* that executes all the individual computations needed to complete a job. The *MedeA* TaskServer gives you several options on how to run your computational tasks, e.g. you can choose to run in serial, in parallel or through a queuing system. You can limit the number of cores used on a specific TaskServer machine. This section describes what options are available to configure how tasks run.

In the following, please have a TaskServer installed that can be contacted through the links **JobServer Home** >> **Administration** >> **TaskServers** or directly through the link <http://<taskserver>:23000> where <taskserver> can be *localhost*, your machine name, or your machine IP address. Both links should open the following page:

Click on the **Administration** tab in the brown navigation bar to proceed to the page with TaskServer configuration options:



This page allows you to manage the TaskServer on this machine. Use the area below to change the settings of parameters that affect how the TaskServer runs. If you want to stop the TaskServer – meaning that no more tasks can be run until it is restarted – use the button at the bottom of the page.

Computing Resources			
Control per number of	Tasks		
Number of Parallel Cores	2	The maximum number of cores per task	Simultaneous tasks
Queue Type	direct		1
			How many tasks to run at once.
			(Apply)
Directories used			
Installation Directory	/home/rshan/MD/2.0		Working Directory
			/home/rshan/MD/2.0/TaskServer
Internals			
Port	23000	The port to listen on (default is 23000).	https
Save files temporarily	<input type="checkbox"/> check to keep temporary task directories for debugging. This is a temporary switch, and will be reset on restarting.		<input type="checkbox"/> Use https rather than the less secure http.
Log Level	notice		Webmaster
			Support@MaterialsDesign.com
(Apply)			
Style Parameters			

The *Control per number of* drop-menu has two options:

- Cores

Follow-up options are:

- *Number of Parallel Cores*: The maximum cumulated number of cores to use for all tasks.
- *Core limit type*: *Hard* or *Soft* which allocates no more than available cores (*Hard*) or if necessary overlaid by maximum 50% (*Soft*).

The **Number of Parallel Cores** determines how many cores are available for all tasks running on this TaskServer. The default, set during installation, is the number of physical cores (no hyper-threading) on the TaskServer. This is the right value for using mpi or direct mode. If you are using an external queuing system you may increase **Number of Parallel Cores** to the number of available cores. The **Number of Parallel Cores** is an upper limit and can be raised at run time in the job submission dialog, which shows the value set for a given queue as the default.

- *Tasks*

Follow-up options are:

- *Number of Parallel Cores*: The maximum number of cores per task.
- *Simultaneous tasks*: How many tasks to run at once.

The *Queue Type* determines how the executables of LAMMPS, GIBBS, VASP, MOPAC, and Gaussian are executed by the TaskServer. The following options are available:

- direct or mpi - uses Intel mpi included in *MedeA* to run parallel jobs.
- *PBS, LSF, GridEngine, etc.* - expects a file `<templateQUEUE>.tcl` in the directory `<md_install_dir>\2.0\TaskServer\Tools\`
 - *PBS* (Linux): works with *PBS, OpenPBS, or Torque*
 - *LSF* (Windows/Unix/Linux)
 - *GridEngine*
 - *SLURM*
 - *LoadLeveler*
 - *manual*: supports running on remote systems with manual transfer

Attention: *MedeA* does not include any of the above queuing systems. You will need to install, configure, and manage the external queuing systems.

In order to run e.g. with *PBS*, copy the file `templatePBS.tcl` to `PBS.tcl` and set the queue type to **PBS** in the TaskServer Administration page. The file `PBS.tcl` provides a number of parameters that can be set to adapt the script to your local environment. The script has to be created for each of the computing codes used, allowing using different queues and other settings for a specific code.

The *Working Directory* is where the TaskServer writes temporary files. This is a scratch directory as all relevant data are exported back to the JobServer upon completion of tasks.

The *Port* is the TaskServer port number. It is not recommended to change the **Port** the TaskServer listens on, unless there is a specific reason for doing so.

The *Save files temporarily* box allows to keep temporary task directories for debugging problems such as submission to the queuing system. Please note that this is a temporary switch and will be reset upon restarting the TaskServer.