Compute cluster guide
TU Darmstadt - Chair of Fluid Dynamic (FDY)

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Abstract: This document explains the usage of the compute cluster at the chair of fluid dynamics, in particular for the execution of BoSSS applications.

1 Notation

$executable The path to the BoSSS binary on your local machine which you want to execute on the cluster

$home `\\fdyprime\usersprace\$yourName\` where `$yourName` is your user name at the FDY

$executionDir An arbitrary sub-directory of `$home` to which the executables will be deployed

$databaseDir The location of a BoSSS database on the server (usually a sub-directory of `$home`)

2 Prerequisites

Before you can run a BoSSS application on the FDY cluster, you need to have the following tools installed on your local machine:

1. BoSSS via an installer from
   `\\fdyprime\bosss\root\install\`
2. Microsoft MPI
   `\\fdyprime\software\microsoft\HPC 2008 R2\ms-mpi`
3. Microsoft HPC Pack R2
   `\\fdyprime\software\microsoft\HPC 2008 R2\`;
   depending on your operating system, either choose the sub-folder
   `Windows HPC Server 2008 R2 win_mac_linux_sun`
   or
   `Windows HPC Server 2008 R2 Suite x64`

In general, both Microsoft tools should already be installed on your machine via OPSI. If not, please contact an administrator.

Additionally, you need a BoSSS database located at `$databaseDir`. If you have not already created one, you can do so by executing the command

```
bcl init-db $databaseDir
```

from a location where you can access bcl.

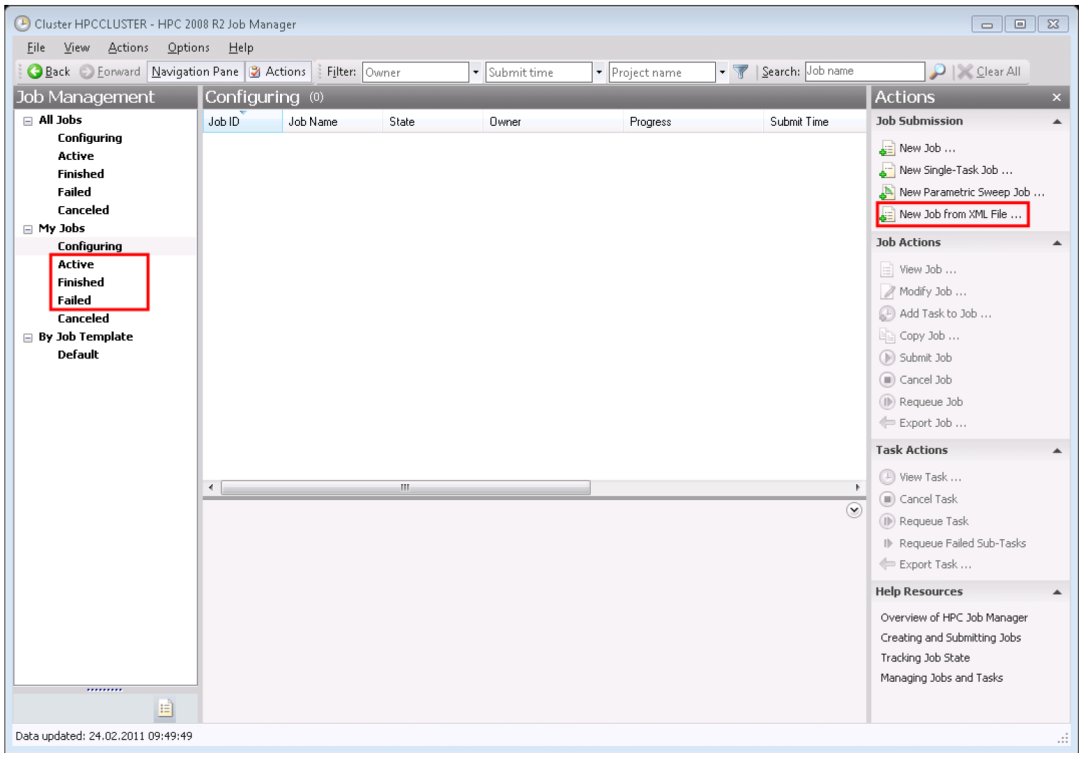

Figure 1: Main screen of the HPC Job Manager

3 Deployment

Before an application can be run on the cluster, it has to be transfered to a location on the server including all its dependencies. You can do by using the

```
bcl deploy-at $executable $executionDir
```

command.

Now, you need to create a control file for you application in `$executionDir$`. The exact content of this file depends on the application but in every case, the path to be database has to be set using the **full** path (see `$databaseDir`).

Finally, the deployment should be done but it is highly recommended to test your deployed application before starting the execution on the cluster. This can simply be done by starting the application in `$executionDir` by hand (possibly with a smaller problem size) and verifying that the initialization completes successfully.

4 Execution

Runs on the FDY cluster can only be initiated by means of the HPC Job Manager. During the first start it will ask you to select a *head node* which in our case simply is `HPCCLUSTER`. For every new run on the cluster you will need to create a new *job*. The easiest way of doing this is to use the template `job-template.xml` which is being distributed with this tutorial. That way, you can use the option *Create New Job from Description File* (see Figure 1) of the Job Manager. Simply select the mentioned file in the dialog and you will be led to the screen displayed in Figure 2 where you can specify a name for the job.

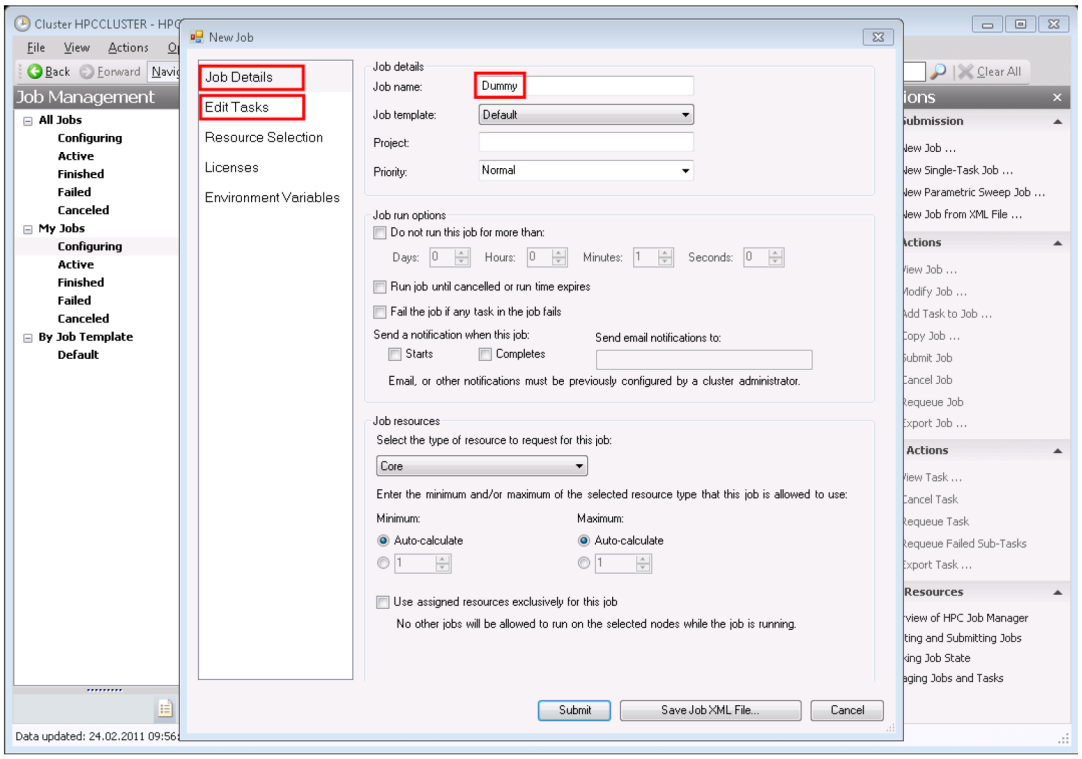

Figure 2: *Create New Job from Description File* dialog

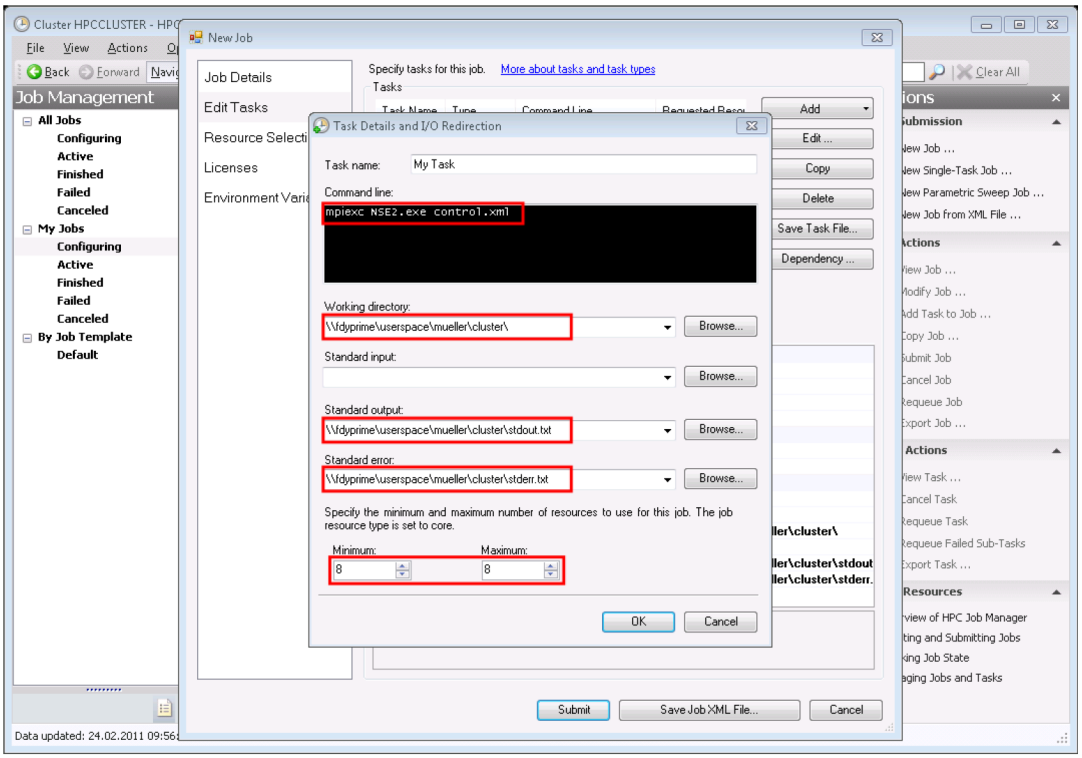

Figure 3: *Edit Task* dialog

Finally, you can proceed to the *task list*. Every run consists of a list of *tasks* which can be specified here. When using the job template mentioned before, one task will already be present. A click on *Edit* will open the screen shown in in Figure 3 where you can specify the task information according to your needs. The most important parts (highlighted in red) are:

Command Line Replace the name of the executable (`NSE2.exe` by default) with the name of your executable (while keeping the `mpiexec` command!). Note that you can explicitly specify the name of a control file as a command line argument to the application if required (e.g. `NSE2.exe -c myControlFile.xml`).

Working directory Replace with the **full** path to `$executionDir`

Standard output Specify the path (either absolute or relative to the working directory) to a file in which you want to store the standard output stream of your program

Standard error Specify the path (either absolute or relative to the working directory) to a file in which you want to store the standard error stream of your program

Number of resources Choose the (minimum and maximum) number of processors you want to use

When you have completed this step you may want to store your settings by means of *Save Job as* in order to be able to reuse your settings for later runs. You are now ready to enqueue your job via *Submit* using your username and your password. You can view the status of your job in the *My Jobs* list in the *Job Management* section of the HPC Job Manager. It will appear in the list of *Active* jobs until it is finished. Afterwards, it will be listed either in the list of *Finished* or *Failed* jobs depending on the outcome of the run.

5 Parametric sweeps

To do