Running MATLAB computations on the Trantor cluster

MATLAB Parallel Server is available on the Trantor cluster, allowing to execute long-running CPU and/or GPU intensive computations on high-performance compute nodes. Furthermore, jobs submission and results retrieval is performed directly from the MATLAB instance running on your personal workstation.

Service availability

In accordance with the terms of the license subscribed by Scuola Normale Superiore, the use of this service is **restricted to SNS students and research staff only**. In addition, access to the service **must be explicitly requested** by writing to hpcstaff@sns.it.

At this time, only the following queues support the execution of MATLAB jobs:

- q07helicon
- q14helicon
- q07daneel
- q14daneel

Please use the 'daneel' queues only if your computation requires GPU hardware.

You can find additional information on the characteristics of these queues and their associated compute nodes on our Website:

https://hpccenter.sns.it/page/wiki/pages/Resources_available_on_Trantor.html https://hpccenter.sns.it/page/wiki/pages/Submitting_Inspecting_and_Cancelling_PBS_Jobs.h tml#Resources_and_queues

Finally remember that the Trantor cluster can be accessed only **within the SNS internal network**. When working offsite, you can establish a VPN connection to the SNS network (see <u>https://ict.sns.it/en/service/access/vpn</u> for details).

License agreement

MathWorks products can be used for **academic purposes only** and their use is subject to the **MathWorks**, **Inc. Software License Agreement and Program Offering Guide**. You can read both documents by selecting the $Help \rightarrow Terms$ of Use menu entry from the MATLAB toolbar, or by opening the file license_agreement.txt stored in your MATLAB installation folder. **Carefully read the terms and conditions before using the software**.

Installing MATLAB on your workstation

- 1. Visit the <u>SNS MathWorks Portal</u>, then click on the "Sign in to get started" button.
- 2. Under the "Campus-Wide Access" section, click the "Get MATLAB access now" button.

- 3. Sign in (if you already have a MathWorks account) or create a new account using your SNS email address.
- 4. In your "*My Account*" page, you should see a "*My Software*" table. Click on the download button on the right side of the row labeled as "*MATLAB (Individual)*". You will be redirected to the "Download" page.

My Softwar	e			
License	Label	Option	Use	
1001009	MATLAB (Individual)	Total Headcount	Academic	€ ×

- 5. Select the **R2022a release**, then download the MATLAB installer for your Operating System. Once downloaded, you can disconnect from the MathWorks portal.
- 6. Run the installer and follow the wizard to install MATLAB on your workstation, signing in with your MathWorks account when required.

Installing the Parallel Computing Toolbox and configuring the cluster integration

The **Parallel Computing Toolbox** plugin provides high-level constructs to parallelize MATLAB programs, allowing to exploit the full processing power of multi-core CPUs and GPUs (refer to the <u>official documentation</u> to learn more). In addition, is it possible to configure the *Parallel Computing Toolbox* to submit computations on a HPC cluster and retrieve the results directly from the MATLAB interface.

Follow these steps to install and configure *Parallel Computing Toolbox* in MATLAB:

- 1. In the toolbar, select the *HOME* tab and click on the *Add-Ons* button. Then, from the *Add-On Explorer* window, install the following plugins:
 - 1.1. Parallel Computing Toolbox
 - 1.2. Parallel Computing Toolbox plugin for MATLAB Parallel Server with PBS



- 2. After installing "*Parallel Computing Toolbox plugin for MATLAB Parallel Server with PBS*", a configuration wizard will start. Follow the guided procedure, answering as follows:
 - 2.1. Q: Select the operating system that your cluster is using A: Unix

Operating System

It is good practice to set up MATLAB on a cluster that is running the same operating system on all cluster machines.

Select the operating system that your cluster is using:

Unix

Windows

2.2. Q: Can your cluster and client machines read and write to a shared job storage location? A: No

Submission Mode

MATLAB provides plugin scripts for three submission modes. Answer the following questions to determine which submission mode is appropriate for your cluster.

Can your cluster and client machines read and write to a shared job storage location? Note: If yes, MATLAB uses the location specified in the JobStorageLocation property of the cluster profile.

O Yes

No

You have selected the nonshared submission mode. The default plugin scripts are located at

- 2.3. Q: Specify the hostname of the cluster submission host A: Insert the FQDN of a head-node, such as trantor02.sns.it
- 2.4. Q: Specify the username to connect to the cluster A: Insert your Trantor account username.
- 2.5. Q: Do you want to use an identity file to log in to the cluster? A: No

Connection Details
Set up additional properties required for the nonshared submission mode.
Specify the hostname of the cluster submission host:
Cluster host: trantor02.sns.it
Specify the username to connect to the cluster:
Username (optional): your username
Do you want to use an identity file to log in to the cluster?
⊖ Yes
⊙ No
Username (optional): your username Do you want to use an identity file to log in to the cluster? O Yes O No

2.6. Q: Specify the location on the cluster to store MATLAB job files for clients A: The program is asking for a temporary folder where to store the data exchanged between the Matlab instance running on your workstation and the workers running on the cluster's compute nodes. We will use a temporary folder in your Trantor home directory for that purpose: /home/<username>/MatlabTmp/

(replace <username> with your actual *Trantor* username).

- 2.7. Q: Use unique subfoldersA: Be sure that the checkbox is checked.
- 2.8. Q: Choose a number of processors per node to use for communicating jobs A: You can leave this field to its default value of **2**. This parameter represents the number of CPU cores per node that Matlab will ask to the scheduling system when submitting a new job. It is preferable to set the actual value for this parameter by code, as discussed in the following.

Cluster Details
Set up additional properties required for cluster configuration.
Specify the location on the cluster to store MATLAB job files for clients:
Remote job storage location: /home/your-username/MatlabTmp/
Use unique subfolders
Select this option to prevent conflicts between jobs submitted from different users and MATLAB versions. MATLAB does this by storing job files in subfolders of the remote job storage location based on client username and MATLAB version.
Choose a number of processors per node to use for communicating jobs:
Processors per node: 2

- 2.9. Q: *Number of workers*A: In our cluster this parameter is just an upper-bound. Set it to **999**.
- 2.10. Q: MATLAB installation folder A: Insert /opt/mathworks/R2022a/
- 2.11. Q: *Number of threads per worker* (under *Advanced configuration*)A: Leave this field to the default value of **1**.

Workers
Job submission requires the following information about workers in your cluster.
Specify the maximum number of MATLAB workers you want to use on your cluster (this must be less than or equal to the maximum number of workers your license supports): Number of workers:
Specify the root folder of the R2022a MATLAB installation for workers (same for all workers): MATLAB installation folder for workers: //opt/mathworks/R2022a/
\sim $ m m m m A}$ Advanced configuration
If your cluster machines have more cores than workers, you can increase the number of computational threads per worker to use all cores on your machines. Note: Performance degrades if the number of computational threads from all workers on a machine exceeds the number of physical cores on the machine.
Number of threads per worker:

2.12. Q: Select the license management that your cluster is using A: Network license manager

License

You must have a MATLAB Parallel Server license that supports the number of workers in your cluster.

Select the license management that your cluster is using:

Network license manager

Online licensing

Other

Select this option for all other license management.

2.13. Q: Specify the name of your profile A: Name the profile '**Trantor**'.

Profile Details
Identify your new profile by giving it a name and an optional description.
Specify the name of your profile:
Profile name: Trantor
Add a short description of the cluster to be included in the profile: Cluster description (optional):

2.14. In the next step, a summary is displayed. Check the inserted values, then press *Create* to save the profile.

- 2.15. Finally, a confirmation dialog appears, asking if you want to set the *Trantor* cluster profile as the new default. It is recommended to leave this checkbox **unchecked**, thus leaving the 'local' profile as default. In fact, **you should develop and debug your program on your machine and resort to the cluster only for long-running computations**.
- 3. Now you need to apply a couple of changes to the scripts of the "*Parallel Computing Toolbox plugin for MATLAB Parallel Server with PBS*" plugin.
 - 3.1. First of all, you need to find where these scripts have been stored. In the toolbar select the *HOME* tab, then click on the *Parallel* \rightarrow *Create and Manage Clusters...* menu entry. The *Cluster Profile Manager* window will appear.



3.2. Select *Trantor* from the *Cluster Profile* list then and the related *Properties* tab, then scroll the form until you find the *SCHEDULER PLUGIN* section. The path where the scripts are stored is given by the *PluginScriptsLocation* property.

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- 3.3. Navigate to this path with your file manager or terminal. You should see the following files (among the others): *independentSubmitFcn.m* and *communicatingSubmitFcn.m*
- 3.4. Download the sample code archive and it. Within the unzip SubmitFunctionsMod folder you will find two files: independentSubmitFcn mod and communicatingSubmitFcn mod. They contain the code to be inserted into *independentSubmitFcn.m* and communicatingSubmitFcn.m (see below).
- 3.5. Open *independentSubmitFcn.m* and find the following line of code:

additionalSubmitArgs = sprintf('-l nodes=1:ppn=%d', numberOfProcs);

Replace this line with the content of *independentSubmitFcn_mod*.

3.6. Open *communicatingSubmitFcn.m* and find the following line of code:

additionalSubmitArgs = sprintf('-l nodes=%d:ppn=%d', numberOfNodes, procsPerNode);

Replace this line with the content of the *communicatingSubmitFcn_mod*.

- 4. It is now possible to 'validate' the profile, so to be sure that the configuration is working properly.
 - 4.1. Open the *Cluster Profile Manager* window again. Be sure to select the *Trantor* cluster profile, then open the *Validation* tab.
 - 4.2. You'll see a list of 'stages' (tests) that can be performed. Select all the stages with the exception of the one named "*Parallel pool test (parpool)*", which must be **unchecked**.
 - 4.3. <u>Set 2 as number of workers</u>.
 - 4.4. Finally, press the *Validate* button to start the tests. After a few seconds, MATLAB will ask you the password for the Trantor cluster.
 - 4.5. All the activated tests should pass.

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Cluster Profile	Trantor					Type: Generic (How	to configure)
local (default)	Properties Validation						
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	Cluster connection test	(parcluster)	Passed				
	Job test (createJob)		Passed				
	SPMD job test (created	CommunicatingJob)	Passed	Job ran with 2 v	vorkers.		
	Pool job test (createCo	ommunicatingJob)	Passed	Job ran with 2 v	vorkers.		
	Parallel pool test (parp	oool)	Ø Skipped	Not included in	validation.		
	Number of workers to use	2 -					
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	No further details for th	is stage.					
						Validate Sh	ow Report

You can start a new cluster profile configuration wizard by executing the following command:

```
parallel.cluster.generic.runProfileWizard()
```

Running MATLAB batch jobs on the cluster

In general, Parallel Computing Toolbox supports two modalities to run computations on a cluster:

- By directly making use of a (local or remote) parallel pool of workers. This modality has the advantage of providing an interactive computing experience (see the <u>parpool</u> function documentation for details).
- By submitting the computation as an "off-line" job by means of the <u>batch</u> function. This modality is primarily designed for long-running tasks. Users can close the MATLAB client while the job is running, and retrieve the results from script once terminated.

Please note that, at this time, **only batch jobs are supported on** *Trantor*. You can however use an interactive parallel pool on your local machine, by selecting the '**local**' parallel profile. This is particularly useful for development purposes.

The following sections discuss the code required to submit a batch job on *Trantor* and to retrieve the results from your scripts.

Job submission and monitoring

First of all, you need to decide the amount of computational resources to request for the job. Let's say you want to run your parallel job with N worker processes. In your script, you can then define the following variable:

workers = N;

Also note that MATLAB Parallel Server also spawns a 'master' process in addition to the workers:

```
processes = workers + 1;
```

The next step is to choose a group of nodes on which to run the computation. You do so by selecting a submission queue:

queueName = '...';

Note

At this time, only the following queues support the execution of MATLAB jobs:

q07helicon

```
Тір
```

- q14helicon
- q07daneel
- q14daneel

Let C be the number of CPU cores available on the nodes you intend to use:

maxCoresPerNode = C;

Since it is advisable to reserve one CPU core for each process, the number of nodes and the amount of cores per node to be requested are given by:

```
coresPerNode = min(processes, maxCoresPerNode);
numberOfNodes = ceil(processes/coresPerNode);
```

You also have to define the amount of RAM memory to reserve on each node:

```
memPerProcess = M;
memPerNode = memPerProcess * coresPerNode;
```

where *M* is the memory to assign to each process, expressed in **GB**.

The next step is to create an instance of the *Trantor* cluster profile (see *parallel.Cluster* documentation for details). The resources requested for the job must then be assigned to the fields of the cluster object:

```
cluster = parcluster('Trantor');
cluster.AdditionalProperties.QueueName = queueName;
cluster.AdditionalProperties.ProcsPerNode = coresPerNode;
cluster.AdditionalProperties.MemPerNode = memPerNode;
cluster.AdditionalProperties.GpusPerNode = 0;
```

Note that:

- The number of compute nodes must not be explicitly set. Instead, it will be automatically computed according to the other parameters.
- You can reserve one or more GPUs per node if your computation requires them. If so, be sure to select a queue whose compute nodes are equipped with GPU hardware.

The actual job submission takes place by calling the *batch* function:

```
batch(cluster, @myFunction, 1, {200}, ...
'Pool', workers, ...
'AutoAddClientPath', false);
```

You should provide at least the following arguments to *batch*:

• The cluster object.

- A reference to the function to be executed on the cluster, the number of return values and the number of arguments.
- The number of workers to employ.
- The assignment of the AutoAddClientPath property to false. This prevents client-related paths from being used by the workers.

On *batch* execution, the following happens:

- 1. The program will ask for your Trantor password.
- 2. A few job data files will be created on your current working directory, as shown by the following screenshot:

 Name ∠ Job8 Job8.metadata.txt Job8.state.mat job_results_retrieval.m job_submission.asv job_submission.m 	Current Folder	۲
 Job8 Job8.in.mat Job8.metadata.txt Job8.state.mat job_results_retrieval.m job_submission.asv job_submission.m mxEunction.m 	🗋 Name 🛆	
Job8.in.mat Job8.metadata.txt Job8.state.mat job_results_retrieval.m job_submission.asv job_submission.m	🗉 🧰 Job8	
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☐ job_submission.asv job_submission.m myEunction.m	🖄 job_results_retrieval.m	
🖆 job_submission.m 👰 myEunction.m	🗋 job_submission.asv	
🖄 myEunction.m	🖄 job_submission.m	
	🖄 myFunction.m	

Do not touch these files!

- 3. The job data files will be uploaded to your *Trantor* home folder, within the *MatlabTmp* directory.
- 4. A job is submitted to the PBS scheduling system.

You can monitor the state of your jobs by opening the *Monitor Job* panel from the *Parallel* menu in the toolbar:



Comma	and Window		Jo	b Monitor		C
Select	Profile: Trantor	-			✓ Show	w jobs from all users
ID	Username	Submit Time	Finish Time	Tasks	State	Description
1	100 C	Thu Apr 28 09:20:50		5	running	Batch job r
Last u	pdated at Thu Ap	r 28 09:21:28 CEST 2022		Auto updat	te: Every 5 minutes	V Update Now

In the Job Monitor panel be sure to select the 'Trantor' profile.

Of course, you can also use the *qstat* utility to monitor your job (see <u>here</u> for details). To this end, you can find the PBS Job ID by right-clicking over the job row and selecting *Show Details* from the contextual menu. The PBS Job ID will be printed on the *Command Window*:

Command Window		\odot
Associated Tasks:		^
Number Pending: 5		
Number Running: 0		
Number Finished: 0		
Task ID of Errors: []		
Task ID of Warnings: []		
Task Scheduler IDs: 85265.pbs01		
fx >>		~
<	>	,

Once the job appears in the *Job Monitor* panel with a **queued or running state**, you can **safely close MATLAB on your local machine**.

Retrieving the job results

Since batch processing on a cluster is designed for long-running jobs, it is common to open MATLAB from time to time to check if the job is still running and, once finished, to retrieve the results.

Once opened MATLAB, you may need to change the current working folder to the directory where the job data files are located (otherwise MATLAB will not be able to recognize the job). Then open the *Job Monitor* panel and change the selected profile to '*Trantor*' (if the *Trantor* profile was already selected, you may need to switch to the *local* profile and then select *Trantor* again). The program will ask you for the password of your Trantor account, then the job's details should appear in the *Job Monitor* panel.

Тір

As explained before, a faster way to check if your job is still running is by using the **qstat** utility. For example, you can execute the following command from your terminal to connect to the cluster, executing *qstat* to print your **running** jobs and then automatically disconnect:

ssh username@trantor02.sns.it qstat -n1 -u username

When the job is finished, you can retrieve the results from script, so to visualize them and/or perform further analysis.

First of all, you need to create a new instance of the 'Trantor' cluster profile:

```
cluster = parcluster('Trantor');
```

Then, use the *findJob* function to (re)create an object representing your job:

```
job = findJob(cluster, 'ID', JOB_ID);
```

where the Job ID is the one shown on the first column of the Job Monitor panel.

To retrieve the results it is sufficient to call the *fetchOutputs* function, passing the job object as argument:

```
results = fetchOutputs(job);
```

Finally, it is important to delete the job, so to clean the residual data files from the current working folder on your local machine and from the temporary directory in your Trantor home:

delete(job);

Sample code

You can download a few examples and the code required by the configuration procedure <u>here</u>. The archive contains the following folders:

- SubmitFunctionsMod : replacement code for the "Parallel Computing Toolbox plugin for MATLAB Parallel Server with PBS" plugin.
- *JobSubmissionAndRetrieval* : this example shows how to submit a long-running job on the cluster and retrieve the results at a later time.
- *GPUsInfo* : this example shows how to retrieve the characteristics of the GPUs that have been reserved on the compute node by means of the *gpuDeviceTable()* function.

Best practices

- Prefer the '*local*' cluster profile during development, since it allows you to develop and test your parallel program in an interactive fashion (on your local machine). Once the codebase is stable, you can then make use of the cluster to speed-up long-running computations.
- If your computation performs I/O intensive operations on files, make use of the local scratch areas available on many compute nodes, as discussed <u>here</u>. Then, at the end of the computation, please remember to copy any relevant file from the

scratch folder back into your home or project folder. In fact, local scratch areas are not backed up and can be erased by the technical staff for maintenance purposes.

• While most of the data files are erased when deleting the job from MATLAB, the program leaves some residues in the *MatlabTmp* folder of your Trantor home. Please **clean up the content of this directory from time to time**. However, be sure that no MATLAB jobs are running when deleting these files.

Further documentation

To learn more about Parallel Computing Toolbox and Batch Processing in MATLAB, please refer to the official documentation:

https://www.mathworks.com/help/parallel-computing/index.html https://www.mathworks.com/help/parallel-computing/batch-processing.html

You can find an introduction to the PBS job scheduler and its use on Trantor at the following Web page:

https://hpccenter.sns.it/page/wiki/pages/Submitting_Inspecting_and_Cancelling_PBS_Jobs.h tml