Getting Started with Parallel Computing using MATLAB on the PARAM Ganga HPC Cluster

This document provides the steps to configure MATLAB to submit jobs to a cluster, retrieve results, and debug errors.

INSTALLATION and CONFIGURATION

The PARAM Ganga MATLAB support package can be found at
https://channeli.in/api/django_filemanager/media_files/49538/

Download the ZIP file and start MATLAB. The ZIP file should be unzipped in the location returned by calling

```
>> userpath
```

Configure MATLAB to run parallel jobs on the cluster by calling `configCluster`. `configCluster` only needs to be called once per version of MATLAB.

```
>> configCluster
```

Submission to the cluster requires SSH credentials. You will be prompted for username and password or identity file (private key). The username and location of the private key will be stored in MATLAB for future sessions.

Jobs will now default to the cluster rather than submit to the local machine.

NOTE: To submit to the local machine instead of the cluster, run the following:

```
>> % Get a handle to the local resources
>> c = parcluster('local');
```

CONFIGURING JOBS

Prior to submitting the job, various parameters can be assigned, such as queue, e-mail, walltime, etc. The following is a partial list of parameters. See `AdditionalProperties` for the complete list. *None of these are required. Refer to the User Manual for more information.*

```
>> % Get a handle to the cluster
>> c = parcluster;

>> % Specify the account
>> c.AdditionalProperties.AccountName = 'account-name';

>> % Specify a constraint
>> c.AdditionalProperties.Constraint = 'feature-name';

>> % Request email notification of job status
>> c.AdditionalProperties.EmailAddress = 'user-id@iitr.ac.in';
```

```
>> % Specify number of GPUs
>> c.AdditionalProperties.GPUssPerNode = 1;
>> c.AdditionalProperties.GPUCard = 'gpu-card';

>> % Specify memory to use, per core (default: 4gb)
>> c.AdditionalProperties.MemPerCPU = '6gb';

>> % Specify the partition
>> c.AdditionalProperties.Partition = 'partition-name';

>> % Specify cores per node
>> c.AdditionalProperties.ProcsPerNode = 4;

>> % Specify the QOS
>> c.AdditionalProperties.QoS = 'qos-name';

>> % Set node exclusivity (default: false)
>> c.AdditionalProperties.RequireExclusiveNode = true;

>> % Use reservation
>> c.AdditionalProperties.Reservation = 'reservation-name';

>> % Specify the wall time (e.g., 1 day, 5 hours, 30 minutes)
>> c.AdditionalProperties.WallTime = '1-05:30';
```

Save changes after modifying AdditionalProperties for the above changes to persist between MATLAB sessions.

```
>> c.saveProfile
```

To see the values of the current configuration options, display AdditionalProperties.

```
>> % To view current properties
>> c.AdditionalProperties
```

Unset a value when no longer needed.

```
>> % Turn off email notifications
>> c.AdditionalProperties.EmailAddress = '';
>> c.saveProfile
```

INDEPENDENT BATCH JOB

Use the `batch` command to submit asynchronous jobs to the cluster. The `batch` command will return a job object which is used to access the output of the submitted job. See the MATLAB documentation for more help on `batch`.

```
>> % Get a handle to the cluster
>> c = parcluster;

>> % Submit job to query where MATLAB is running on the cluster
>> job = c.batch(@pwd, 2, {}, 'CurrentFolder','.');

>> % Query job for state
>> job.State

>> % If state is finished, fetch the results
>> job.fetchOutputs{:}

>> % Delete the job after results are no longer needed
>> job.delete
```

To retrieve a list of running or completed jobs, call `parcluster` to return the cluster object. The cluster object stores an array of jobs that are queued to run, are running, have run, or have failed. Retrieve and view the list of jobs as shown below.

```
>> c = parcluster;
>> jobs = c.Jobs
>>
>> % Get a handle to the second job in the list
>> job2 = c.Jobs(2);
```

Once the job has been selected, fetch the results as previously done.

`fetchOutputs` is used to retrieve function output arguments; if calling `batch` with a script, use `load` instead. Data that has been written to files on the cluster needs be retrieved directly from the file system (e.g., via sftp).

```
>> % Fetch all results from the second job in the list
>> job2.fetchOutputs{:}
```

PARALLEL BATCH JOB

`batch` can also submit parallel workflows. Let's use the following example for a parallel job, which is saved as `parallel_example.m`.

```
function [sim_t, A] =
parallel_example(iter)

if nargin==0
    iter = 8;
end

disp('Start sim')

t0 = tic;
parfor idx = 1:iter
```

```
    A(idx) = idx;
    pause(2)
    idx
end
sim_t = toc(t0);

disp('Sim completed')

save RESULTS A

end
```

This time when using the `batch` command, also specify a MATLAB Pool argument.

```
>> % Get a handle to the cluster
>> c = parcluster;

>> % Submit a batch pool job using 4 workers for 16 simulations
>> job = c.batch(@parallel_example, 1, {16}, 'Pool',4, ...
       'CurrentFolder','.');

>> % View current job status
>> job.State

>> % Fetch the results after a finished state is retrieved
>> job.fetchOutputs{:}

ans =

     8.8872
```

The job ran in 8.89 seconds using four workers. Note that these jobs will always request N+1 CPU cores, since one worker is required to manage the batch job and pool of workers. For example, a job that needs eight workers will request nine CPU cores.

Run the same simulation but increase the Pool size. This time, to retrieve the results later, keep track of the job ID.

NOTE: For some applications, there will be a diminishing return when allocating too many workers, as the overhead may exceed computation time.

```
>> % Get a handle to the cluster
>> c = parcluster;

>> % Submit a batch pool job using 8 workers for 16 simulations
>> job = c.batch(@parallel_example, 1, {16}, 'Pool',8, ...
       'CurrentFolder','.');

>> % Get the job ID
>> id = job.ID
```

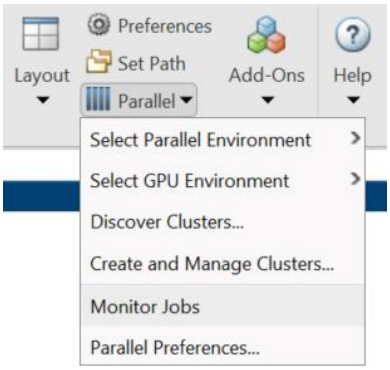
```
id =

     4

>> % Clear job from workspace (as though MATLAB exited)
>> clear job
```

With a handle to the cluster, the `findJob` method searches for the job with the specified job ID.

```
>> % Get a handle to the cluster
>> c = parcluster;

>> % Find the old job
>> job = c.findJob('ID', 4);

>> % Retrieve the state of the job
>> job.State

ans =

     finished

>> % Fetch the results
>> job.fetchOutputs{:};

ans =

     4.7270
```

The job now runs in 4.73 seconds using eight workers. Run code with different number of workers to determine the ideal number to use.

Alternatively, to retrieve job results via a graphical user interface, use the Job Monitor (Parallel > Monitor Jobs).



HELPER FUNCTIONS

Function	Description
clusterFeatures	List of cluster features/constraints

clusterGpuCards	List of cluster GPU cards
clusterPartitionNames	List of cluster partition
disableArchiving	Modify file archiving to resolve file mirroring issue
fixConnection	Reestablish cluster connection (e.g., after reconnection of VPN)
willRun	Explain why job is queued

DEBUGGING

If a serial job produces an error, call the `getDebugLog` method to view the error log file. When submitting an independent job, specify the task.

```
>> c.getDebugLog(job.Tasks)
```

For Pool jobs, only specify the job object.

```
>> c.getDebugLog(job)
```

When troubleshooting a job, the cluster admin may request the scheduler ID of the job. This can be derived by calling `getTaskSchedulerIDs` (call `schedID(job)` before R2019b).

```
>> job.getTaskSchedulerIDs()

ans =

      25539
```

TO LEARN MORE

To learn more about the MATLAB Parallel Computing Toolbox, check out these resources:

- Parallel Computing Coding Examples
- Parallel Computing Documentation
- Parallel Computing Overview
- Parallel Computing Tutorials
- Parallel Computing Videos
- Parallel Computing Webinars