# Parallel Horace – design ideas

## User interaction.

1. A user expected to continue to use Horace as he does now, i.e. typing or scripting Horace commands.
2. If appropriate powerful machine or parallel cluster is available to a user, user would enable parallel capabilities by issuing a simple command. (e.g. **hpc on**), which spawns execution of the time consuming operations in parallel.
3. The parallel Horace’s features are configured using Herbert configuration classes and available for advanced users to configure and fine-tune. A simplified default version of the framework should run without any users configuring.
4. User may or may not have access to parallel computing toolbox and distributed Matlab server. The presence to these resources improves user’s computational capabilities, but the basic access to parallel Horace resources expected to be independent on these resources.
5. The commands which may take long time and will benefit from parallelization are **gen\_sqw cut\_sqw**, **unit** and **binary operations**, **tobyfit.fit** ,**sqw\_eval** and **symmetrise**.

## Technical facts, constrains and opportunities.

1. All Horace algorithms benefiting from parallelization can be summarized by the following pseudocode:

*while* condition(Data):

*For* i=1:N\_iterations

Results(i) = Do\_processing(Data,i)

*End*

condition,summary =

reduce\_results\_process\_condition(Data,Results)

*end* (condition)

*return* summary

where expensive operations of interest on Data are in fact the operations over the pixels of one or the group of sqw objects. The sqw objects expected not fit the memory. The *Do\_processing* operation can be efficiently executed independently on each pixel or small group of pixels located im memory or retrieved from a file system while *reduce\_results\_process\_condition* request interprocess communications. The condition and summary variables can easy fit the memory of a single node and exchanged through MPI communications.

The sufficient way for parallelizing such job would be division of the Data in the *For* loop among MPI workers and the usage of MPI communications to gather Results and condition on a head MPI node.

1. A MPI job can always and only be executed in the form:

>> mpiexec n\_workers the\_mpi\_program

1. Matlab supports MPI jobs submitting parallel task to a ***cluster*** :

*cl = parcluster();*

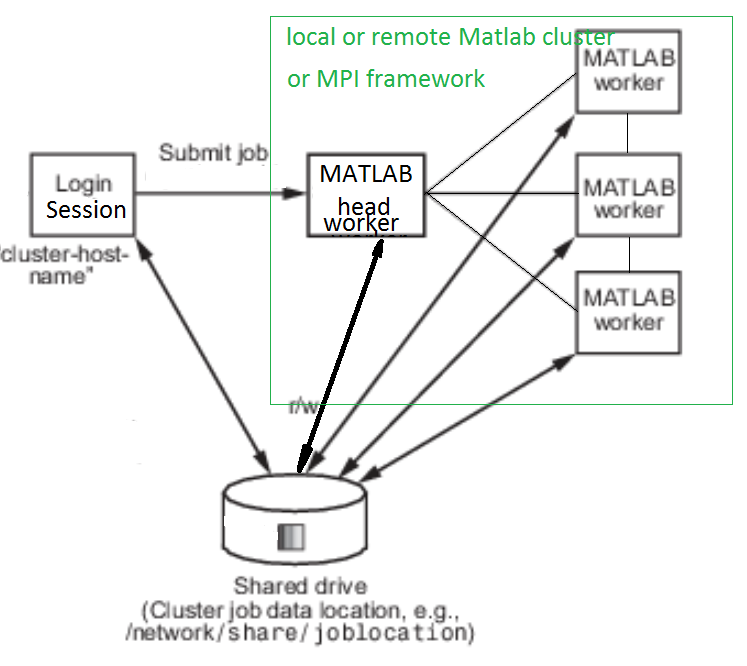
cjob = createCommunicatingJob(cl,'Type','SPMD');

task = createTask(cjob,UserFunctionHandle ,0,{user\_function\_inpts});

submit(cjob);

where the **submit** function is equivalent to the start of mpiexec function and number of workers (***n\_workers***) is defined previously within a ***cluster*** configuration (***n\_workers*** = cl.NumWorkers)

1. The Matlab ***cluster*** configuration necessary and sufficient to run Horace MPI jobs 2.1 above has the form:



1. We expect to design and create software, working in 3 main hardware/software configurations:
   1. A powerful user machine with or without parallel computing toolbox powerful enough to run number of headless Matlab sessions and accessing fast file system.
   2. A user machine with parallel computing toolbox installed and connected to a parallel file system and accessing Matlab distributed computing server installed on a parallel cluster (like SCARF or number of DaaaS virtual machines)
   3. A user function compiled on Matlab with Horace using Matlab compiler and deployed as part of an MPI job on a parallel cluster having compiled Horace installed on each node.

All these configurations can be united under the logical configuration 4)

1. Matlab parallel computing toolbox and distributed Matlab server provide range of classes and functions (blocks) to deliver system independent operations. The blocks we are decided to use are :
   1. parcluster (parpool?) -- provides interface to physical resources and job control operations
   2. MPI commands (e.g. labnum, labsend, labreceive etc), working in a spmd block only and providing low level communication and synchronization routines between different Matlab workers.
   3. SPMD blocks itself, hiding the procedure of task splitting and MPI jobs dispatching on the selected parcluster.

We are going to wrap these blocks into custom classes with common interface, to allow Horace user experience to be independent on presence of parallel computing toolbox and distributed server. The only difference should be in the performance of different configurations.

## Desighn choices.

Set of polymorphic classes will be developed to satisfy user requests 1) with the conditions 2) to support three user cases, namely:

a) User has parallel computing toolbox.

b) User have powerful machine without parallel computer toolbox

c) User has access to cluster where compiled Horace is installed

These classes are:

1. cluster : the interface to parpool class in case a), or the class which supports starting and managing the Matlab workers (headless Matlab sessions) on local machine case b) or MPI framework configurator and interface to mpiexec and MPI framework configuration in the case c)
2. MPI\_communicator: the wrapper for Matlab MPI commands in case a) , or class writing files to be interpreted as MPI messages in case b) or Matlab wrapper around mex file providing access C++ MPI framework in case c).
3. Job\_executor – the abstract class providing access to *Do\_processing* and *reduce\_results\_process\_condition* methods from chapter 2.1. Each supported algorithm from 1.5 would implement this class and provide its own algorithm specific implementations for these methods.
4. Job\_dispatcher – the class which execute Job\_executor’s *Do\_processing*  and *reduce\_results\_process\_condition* methods depending on parallel framework settings and resources, available to user
5. An sqw object and set of sqw objects will get *get\_pixels* method, which would provide access to specified number of pixels out of range of all pixels present in sqw object or sqw objects set regardless of these objects physical location (in memory or in a file)

Finally, a parallel\_config class would allow switching between all these three configurations fine-tuning of the configurations and access to the parameters of these frameworks.

## Note

Only options 3.a and 3.b would be implemented from the beginning of the project. Option 3.c will be implemented if sufficient resources are available.

## Current (01/01/2018) Implementation:

On the date specified in the header, three substantially different blocks of code are written to support the Horace parallel capabilities namely:

1. Herbert Cluster, running multiple Matlab sessions to perform parallel job and using message files to exchange data between workers (Poor-man MPI).

*Its advantages:*

a) No need in parallel computing toolbox and additional Matlab licences

b) The code is fully controlled by Horace development group and can be if necessary extended to provide MPI and cluster capability with no licensing cost (but substantial development cost)

*Its disadvantages:*

1. Runs only on a single node.
2. Becomes extremely slow if an algorithm needs active inter-process communications.
3. Matlab (parpool) cluster running multiple Matlab sessions using Matlab parallel computing toolbox and embedded Matlab MPI intercommunications. Fails back to filebased messages exchange mechanism in case of Matlab MPI being not enabled.

*Its advantages:*

1. Fast (MPI-defined) interprocess communication allowing to run the whole range of Horace algorithms (see below)
2. The possibility to run on a multi-node machine with nodes connected by MPI link or on a parallel cloud if appropriate licenses are available

*Its disadvantages:*

1. Needs parallel computing toolbox license to run on a single node and additional licenses to run on a cluster or cloud
2. The root of developing code without Matlab and additional licenses is completely closed
3. C++ code used to combine binary sqw files into single sqw file

*Its advantages:*

1. Extremely fast and efficient in its area of applicability.
2. With substantial development and inclusion of 3rd party code (Mantid fake MPI (Simon Heybrock private communication) or https://www.codeproject.com/articles/1092727/asynchronous-multicast-callbacks-with-inter-thread) may become a communication hub for the Herbert cluster, overcoming its current disadvantages.

*Its disadvantages:*

1. Currently have very narrow applicability area
2. Has bugs so fails sometimes and currently does not work on SCARF (bugs)
3. C++ code – high cost of development.

As the majority of commonly used Horace algorithms are limited by file-IO speed, one needs fast parallel file system to gain advantage of Horace parallel capabilities.

In additional to that, Herbert Cluster needs powerful multiprocessor machine with multiple processors to run multiple Matlab sessions (At least 64 computational threads and 0.25Tb memory to fully accelerate gen\_sqw on current parallel file system or more if a symmetrisation during file generation is neded.

A Matlab Cluster (parpool) needs either similar machine + parallel computing toolbox licence for each user or multiple nodes connected by parallel file system and fast MPI link + the same toolbox and + Matlab distributed server licenses for each node.

The Horace algorithms and their benefits form each approach are summarized in the table below:

|  |  |  |  |
| --- | --- | --- | --- |
| Algorithm | Herbert Cluster | Parpool cluster | C++ code |
| Gen tmp files (part of gen\_sqw) | 10-fold acceleration | 10-fold acceleration | N/A |
| write\_nsqw\_to\_sqw  (as part of gen\_sqw or separate) | 4-fold deceleration wrt. to serial Matlab code | Substantial acceleration (needs further testing for numbers) | 5-10 fold acceleration |
| Accumulate headers  (as part of gen\_sqw) | Substantial acceleration, a bit slower than Parpool | Substantial acceleration | Currently N/A |
| Accumulate cut (developing) | 10-fold acceleration expected | 10-fold acceleration expected | N/A |
| sqw\_eval (planned development) | n-workers acceleration expected | n-workers acceleration expected | N/A |