HPCC How to run R jobs on Hrothgar



High Performance Computing Center Texas Tech University

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1. Introduction

R Job introduction R is a software package especially suitable for data analysis and graphical representation. Functions and results of analysis are all stored as objects, allowing easy function modification and model building. R provides the language, tool, and environment in one convenient package.

It is very flexible and highly customizable. Excellent graphical tools make R an ideal environment for EDA (Exploratory Data Analysis). Since most high level functions are written in R language itself, you can learn the language by studying the function code.

2. Setting up the environment

Hrothgar is equipped with SoftEnv to set up the environment with minimum work by users. The use of SoftEnv is not required but highly recommended by HPCC staff.

Step 1: setting up user environment

If the user environment is already set up, please skip this step.

At the first use, the user should copy two sample dot-files: dot-bashrc is the start up script which evokes SoftEnv; dot-soft contains a list of software whose specific environment variables will be set up for the user.

\$ cp /lustre/work/apps/examples/dot-bashrc .bashrc
\$ cp /lustre/work/apps/examples/dot-soft .soft
\$ ln -s .bashrc .bash_profile

Log out and log in again.

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👔 Quick Connect 🦳 Profiles	
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-bash-3.2\$ pwd	-
/home/pmane	
-bash-3.2\$ ls -al	
total 60	
drwxr-xr-x 4 pmane CS 4096 Jul 13 13:36 .	
drwxr-xr-x 430 root root 12288 Jul 12 08:35	
-rw 1 pmane CS 15117 Jul 13 12:16 .bash_history	
drwxr-xr-x 12 root root 4096 Jul 13 11:47 examples	
-rw 1 pmane CS 1675 Jul 2 2009 pmane_id	
-rw-rr 1 pmane CS 408 Jul 2 2009 pmane_id.pub	
drwx 2 pmane CS 4096 Jul 6 2009 .ssh	
-rw 1 pmane CS 5783 Jun 8 16:49 .viminfo	
-rw 1 pmane CS 192 May 5 20:15 .Xauthority	
-bash-3.2\$ cp /lustre/work/apps/examples/dot-soft .soft	
-bash-3.2\$ cp /lustre/work/apps/examples/dot-bashrc .bashrc	
-bash-3.2\$ <mark>ln -s .bashrc .bash_profile</mark>	
-bash-3.2\$ ls -al	
total 64	
drwxr-xr-x 4 pmane CS 4096 Jul 13 13:45 .	
drwxr-xr-x 430 root root 12288 Jul 12 08:35	
-rw 1 pmane CS 15117 Jul 13 12:16 .bash history	
lrwxrwxrwx 1 pmane CS 7 Jul 13 13:45 .bash_profile -> .bashrc	
-rwxr-xr-x 1 pmane CS 522 Jul 13 13:44 .bashrc	
drwxr-xr-x 12 root root 4096 Jul 13 11:47 examples	
-rw 1 pmane CS 1675 Jul 2 2009 pmane_id	
-rw-r 1 pmane CS 408 Jul 2 2009 pmane 1d.pub	
-rwxr-xr-x 1 pmane CS 226 Jul 13 13:44 .soft	
arwx 2 pmane CS 4096 Jul 6 2009 .ssh	
-rw 1 pmane CS 5783 Jun 8 16:49 .Viminio	-
-rw 1 pmane CS 192 May 5 20:15 .Xauthority	-
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Step 2: setting up R environment

The latest version of R is installed on Hrothgar. Use the following commands to add R in SoftEnv:

\$ soft add +R \$ which R

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3. Job Submission

3.1. Script for job submission

The following is a script file to submit a R job to hrothgar. The sample script and input files are available at the directory /lustre/work/apps/examples/R. Use the command to copy the directory:

\$ cp -r /lustre/work/apps/examples/R R

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hrothgar:\$ cp -r /lustre/work/apps hrothgar:\$ cd R hrothgar:/R\$ 1s ArrayJob.sh Serial_R.sh hrothgar:/R\$	s/examples/R R	▲
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Below is the example script for ArraJob.sh

#!/bin/bash
#\$ -S /bin/bash
#\$ -t 1-300:1
#\$ -cwd
#\$ -cwd
#\$ -V
#\$ -q serial
#\$ -P hrothgar
/lustre/work/apps/R/bin/R --vanilla < code.\$SGE_TASK_ID >
code.\$SGE_TASK_ID.out

Below is the example script for Serial_R.sh

#!/bin/sh
#\$ -V
#\$ -cwd
#\$ -S /bin/bash
#\$ -N RJOB
#\$ -o \$JOB_NAME.o\$JOB_ID
#\$ -e \$JOB_NAME.e\$JOB_ID
#\$ -q serial
#\$ -P hrothgar

/lustre/work/apps/R/bin/R --vanilla < ds_gfdl_tmax.r > out.118

3.2. Job submission

\$ qsub ArrayJob.sh - To submit your R job to Hrothgar \$ qsub Serial_R.sh

\$ qstat – To check the status of the job

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hrothgar:/R\$ qsub Serial_R.sh Your job 112838 ("RJOB") has been submitted hrothgar:/R\$ qstat	*
job-ID prior name user state submit/start at queue slots ja-task-ID 	
112838 0.00000 RJOB pmane qw 12/08/2010 15:55:28 1	
hrothgar:/R\$ ls	
ArrayJob.sh RJOB.e112838 RJOB.o112838 Serial_R.sh hrothgar:/R\$	
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4. RMPI

4.1. Introduction

RMPI is an interface to MPI that allows R users to take advantage of MPI functionality, without having to learn C, C++ or Fortran.

4.2. Setting up RMPI environment

To run Rmpi jobs you will need a certain R profile. To use the correct R profile, use the following commands to copy the R profile to your working directory:

\$ mkdir \$HOME/R

\$ cp /lustre/work/apps/examples/R/Rprofile \$HOME/R/.Rprofile

Once you have copied the profile you can check if it is in the right directory by using:

\$ Is -a



4.3. Submitting RMPI Jobs

Now that the environment is set up, you can submit a test script. Copy the example files with the following commands:

\$ cp /lustre/work/apps/examples/R/RMPI_Test.R \$HOME/R/RMPI_Test.R

\$ cp /lustre/work/apps/examples/R/RMPI_Job.sh \$HOME/R/RMPI_Job.sh

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Below is the example for RMPI_Job.sh

#!/bin/sh
#\$ -V
#\$ -cwd
#\$ -S /bin/bash
#\$ -N R_par
#\$ -o \$JOB_NAME.o\$JOB_ID
#\$ -e \$JOB_NAME.e\$JOB_ID
#\$ -q normal
#\$ -pe fill 24
#\$ -P hrothgar

mpirun –np 24 /luster/work/apps/R/bin/R –no-save –q < RMPI_Test.R > RMPI_Test.out

Below is the example for RMPI_Test.R

mpi.remote.exec(paste(Sys.info()[c("nodename")],"checking in as",mpi.comm.rank(),"of",mpi.comm.size()))
mpi.close.Rslaves()
mpi.quit()

\$ qsub RMPI_Job.sh - To submit RMPI job

\$qstat - To check job status

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For Additional Assistance Contact: <u>hpccsupport@ttu.edu</u>

For Comments/Suggestions on user guide <u>hpcc@ttu.edu</u>

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