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Research Computing > First time submitting a Casper job

CUSTOMER WAIT

First time submitting a Casper job (RC-15406)

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Derek Pierson
Creator

Brett Neuman

ACTIVITY

Derek Pierson

17/Oct/22 10:46 AM LATEST

Thanks Dick. I was able to complete enough model runs yesterday to move forward with data analysis. I feel like I have at least a basic understanding of running jobs on Cheyenne now, so I should be good to go from here. Thank you so much for your help!

Richard Valent 16/Oct/22 8:07 PM

Hi Derek;

Your final "batch_MIMICS" job today 6896372 ran for about 30 minutes, using 32 processors. It was not run on a large-memory node. It looks like it was successful.

I'll stay posted intermittently today and partly tomorrow, in case you have further questions.

Best, --Dick

Richard Valent 16/Oct/22 2:28 PM

Hi Derek; you are welcome. Sounds like a good prognosis for your jobs!

As far as I know, there's no PBS-sanctioned way to submit a job multiple times.

You can do this simply via the command line

```
qsub job; qsub job; qsub job;
qsub job; qsub job
```

Or via a bash script using the "for' command.

```
#!/bin/bash
for i in {1..5}
do
   qsub job
done
```

That said, I will return around six pm MDT. Cheers! --Dick

Your request status changed to: **Customer wait** 16/Oct/22 2:28 PM

Derek Pierson 16/Oct/22 1:29 PM

Thanks for all of your help Dick! Looks like I should have no problem getting to 500,000 runs today. That should be enough to proceed with the next phase of data analysis and then come back for to do more runs as needed.

Indeed it looks like I hit the memory limit on that first large run. Looks like my current script with 50,000 runs is right in the

sweet spot, using ~40 gb of memory.

With the qsub command, is there any way to request that I want it do the job n times? Is that an appropriate practice?

e.g. qsub job * 5

I greatly appreciate your help this morning. I'm all set for the week ahead, so no rush on these replies.

Derek

Your request status changed to: **Support wait** 16/Oct/22 1:29 PM

Your request status changed to: **Customer wait** 16/Oct/22 12:52 PM

Richard Valent

16/Oct/22 12:52 PM

Hi Derek; answering your memory-limit question:

The usable memory limit on a small-memory Cheyenne node (the default) is about 45GB.

You can get 109GB by specifying a large-memory Cheyenne node as follows:

```
#PBS -l
select=1:ncpus=36:mpiprocs=36:m
```

PS I will be checking our communications intermittently for about the next 1.5 hours i.e. until ~2:15 MDT. Then I will be away from my terminal until ~6:15 MDT

at which point I will resume checking communications.

Derek Pierson

16/Oct/22 11:36 AM

Running a set of 50,000 did work (previous failed run was set to 100,000).
Below is the output I received by email. Do you know the memory limit?

PBS Job Id: 6893123.chadmin1.ib0.cheyenne.ucar.edu
Job Name: batch_MIMICS
Execution terminated
Exit_status=0
resources_used.cpupercent=3126
resources_used.cput=09:11:13
resources_used.mem=40689060kb
resources_used.ncpus=32
resources_used.vmem=47526760kb
resources_used.walltime=00:29:45

Derek Pierson

16/Oct/22 10:49 AM

Larger run ran into some sort of bus error. See attached log. Could this be a memory issue?
Assuming I can work around this for the time being by submitting multiple smaller jobs...

batch_MIMICS.o6892700

Your request status changed to: **Support wait** 16/Oct/22 10:49 AM

Your request status changed to: **Customer wait** 16/Oct/22 10:27 AM

Richard Valent

16/Oct/22 10:27 AM

Derek, this sounds like great scaling!

It looks like you are running Cheyenne batch jobs.
Congratulations and Hooray!

Let me know if further questions.

--Dick

PS I'll be away from my terminal for an hour or so. Need to get some exercise. Cheers!

Your request status changed to: **Support wait** 16/Oct/22 9:57 AM

Derek Pierson 16/Oct/22 9:57 AM

Parallel improvement looks good. Proceeding to a much larger job.

Test of 1000 model runs (200,000 steps):
7 cores --> 98.5 sec
15 cores --> 46.98 sec
31 cores --> 24.9 sec

Richard Valent

16/Oct/22 9:44 AM

Hi Derek; you've made a common and understandable mistake.

The penalty does not include banishment, only session loss. You'll have received an email

saying this (I also receive a copy and have looked at it.)

Please go ahead and log back in to Cheyenne. You should be able to do that without trouble. When convenient, modify the batch job I provided and submit it.

Let me know how it goes. Best regards. --Dick

PS Sounds like you're getting the expected scaling. That's great!

Your request status changed to: **Customer wait** 16/Oct/22 9:44 AM

Derek Pierson 16/Oct/22 9:41 AM

Nevermind the previous reply. The system let me back in.
I just submitted a job and it worked! I'm moving on to testing/ramping up the processing speed.

Derek Pierson 16/Oct/22 9:28 AM

Well, I made an oopsy. I was doing one last test on the login node and I forgot to cut my number of cores down in the R script. The script drew on 71 cores for ~15 sec. As I'd expect, itlooks like I have been banned by the system. What is the process to get access restored? I won't do it again, scouts honor.

The job file is very helpful. After one last test of my Rscript (~1 min run time) to make certain everything is working, I'll submit a test job.

Your request status changed to: **Support wait** 16/Oct/22 9:28 AM

Your request status changed to: **Customer wait** 15/Oct/22 5:23 PM

Richard Valent 15/Oct/22 5:23 PM

Hi Derek; you are welcome, for the October 17-20 downtime reminder.

Answering your question **Can I achieve this same sort of workflow with a job script?** There should be no problem doing so.

For Cheyenne, I've prepared a simple sequential R hello_world batch job for you to adapt to your needs:

```
/glade/scratch/valent/dpierson/
```

Please copy it to one of your directories, and change it as you wish. Submit it from Cheyenne like this:

```
qsub job
```

The output will be returned in the directory from which you submitted the job.

You might want to do some quick scaling trials to make sure your job running in parallel. I.e. to run it on ten processors, use this directive below instead of the "36" one in the job I've given you:

```
#PBS -l
select=1:ncpus=10:ompthreads=10
```

Then follow with a job on 20 processors, to see if 20 is faster than 10 is faster, as expected.

I will have some dinner soon, but will check for your communication shortly thereafter.

Best, --Dick

Your request status changed to: **Support wait** 15/Oct/22 12:05 PM

Derek Pierson

15/Oct/22 12:05 PM

Thanks for the note about the down time next week. Cheyenne is where I have been running my test script thus far (R script, not openMD). All I've done to use R on Cheyenne is load the R/4.1.3 module, then launch R (installed a couple packages the first time), and then source the test script from within R. Can I achieve this same sort of workflow with a job script? e.g. request 1 node with 36 proc >> load R module >> run R script

One node with 36 proc should work just fine. I can adjust the number or model runs to keep within the wall time, though I don't expect to pushing the 12 hour limit. So perhaps Cheyenne is the way to go?

Richard Valent 14/Oct/22 7:56 PM

Hi again, Derek; I have one more comment:

Next week Oct 17-20 we're down for systems maintenance as per arc.ucar.edu/articles/328.

I'll check this ticket intermittently this weekend in case you have questions and are trying to run your job. I'll do my best to answer as soon as possible but there will be delays since it is the weekend.

Best. --Dick

Your request status changed to: **Customer wait** 14/Oct/22 5:08 PM

Richard Valent 14/Oct/22 5:08 PM

Derek, you are welcome.

The only question I had, is whether OpenMP integrates with the R codes. Is the code you're running an OpenMP code? If not, keep reading ...

If you want to run across more processors, similar to what you were doing on the login node, I'd suggest the **excccasper** command. Using it, you can specify the time duration (up to 24 hours) and also the number of cores you need.

I wouldn't suggest more cores than 8 per node on Casper, because those nodes are meant to be shared. However, we can make an exception if there is a cogent reason.

Also, you might consider running your job on Cheyenne, where you can easily request 36 processors

per node. On Cheyenne you would use a different command (qinteractive or qcmd) and that should work fine though you will only get 12 hours walltime there.

Let me know your thoughts about this. It sounds like you are pretty close to running, with the test jobs you've already made.

Your request status changed to: **Support wait** 14/Oct/22 4:52 PM

Derek Pierson 14/Oct/22 4:52 PM

Thanks for you help Richard. I've been through the R parallel documentation before, though I'm admittedly not an expert. It's been so long now I forget why I moved away from the parallel package to furrr. I think it may have been simply for the pipes (i.e. keeping in the Hadley Wickham universe). Perhaps this application is somewhat unique in that a single model step is quick, but the number of steps I need to make for this monte carlo parameterization scheme is huge (2.4 billion).

The R scripts are set up intentionally, to allow for varied applications without having to refactor the code. This helps us avoid errors, make quick updates, and reuse the model code across projects.

Can you elaborate on the issue you've found with the R scripts I sent? We have used previous versions on other HPC clusters with great success. Quick testing on the Cheyenne login node shows that

without the parallelization, 200,000 model steps take ~9 minutes, a multisession plan takes 46 sec, and a multicore plan takes 22 sec. Using multicore, my estimated completion time for the full 2.4 billion steps would then be ~6 hours.

Richard Valent 14/Oct/22 4:35 PM

Derek, one more thought as we approach the weekend:

If there are no dependencies between the parallel R processes you want to run, a very simple approach is to run each of them as a separate sequential job, then combine the outputs after they have completed.

Many of our users run this way, as opposed to providing a harness that hooks all the processes together, as is needed when the processes are not independent. But it is much more complex and time consuming than if you are a scientist or researcher running experiments with independent processes that need to run in parallel.

Again, let me know your thoughts about the approach you think might work best for you. Especially if you have questions.

Your request status changed to: **Customer wait** 14/Oct/22 3:48 PM

Richard Valent 14/Oct/22 3:48 PM

Thank you, Derek. At this time, I think zoom is premature. I am still

gathering information from you. I do that best in this ticket format, though I realize it is tedious.

I have briefly examined the three R scripts. Below are my answers. After you have read them, and studied the parallel-computation document I've cited below, let me know your thoughts.

```
Q1. Is an OpenMP_job
appropriate? I just need to
run an R script and write
the output.

A1. I am guessing an OpenMP
job is not appropriate,
because it assumes you have
a Fortran or C code
underlying your R code,
i.e.tying its individual
processes together.
Rather, I am thinking that
you want to stay in the R
domain rather than mixing
languages like R and
Fortran or C.  I believe
this document explains the
direction you want to be
heading
https://bookdown.org/rdpeng/
```

Derek Pierson 14/Oct/22 2:52 PM

MIMICS_repeat_base.R
MIMICS_INC_daily.R

Derek Pierson 14/Oct/22 2:51 PM

Absolutely. Good timing as I'm working out some final details in the scripts right now.

There are three R scripts involved. (code is separated only to keep things compartmentalized)
1)The base ftn for running a single iteration of the MIMICS model

(currently set up to simulate a soil incubation over 200 days)

2) A repeat function to run the model for each row of the input data set and compile the output.

3) A script that run the repeat function using n random parameterization sets and compile the output. This is the script that is set up to run in parallel.

If it's easier to jump on Zoom and chat, just let me know. I can send a link.

Thanks for you help!

MSBio_MIMICS_MC_run.R

Your request status changed to: **Support wait** 14/Oct/22 2:51 PM

Your request status changed to: **Customer wait** 14/Oct/22 2:35 PM

Richard Valent 14/Oct/22 2:35 PM

Hi Derek; thank you for asking advice **on first time submitting a job to Casper**.

Before answering your nicely-stated five questions, I'd like to see the R script and supporting code that you have written. Seeing it may help me assist you quicker and better.

If my request is premature, i.e. at this point you are gathering information for putting the code together, let me know that and I will address the questions,

although in doing so I might need to ask you a few questions in return.

Sound OK? --Dick Valent, NCAR Consulting Services Group

Derek Pierson 14/Oct/22 1:45 PM

MSBio_Job_1-1.txt *(0.3 kB)*

DETAILS

Details

Username: dpierson
Projects: p93300641

Hi,

I'm working on parameterization of the MIMICS model for a project with Will Wieder and I'm looking to submit a job on Casper. I've read through the documentation online, but I'm still a bit unsure of the process. I've tested an abbreviated version of the parameterization script (R script) on a login node and I'm ready to submit the full job. Would it be possible to setup a short call (zoom?) to run through the basics of submitting a job? I'm guessing that might prove to be easier than going back and forth by email or the trial and error route.

I've attached the job file I've modified from the online template. I have a few questions:

Is an OpenMP_job appropriate? I just need to run an R script and write the output.
Do I need to do anything to in the job script to load R? Point to packages?
Will the working drive be set to the directory I launch the job script from?
I'd to like use as many cores as I can on one node. What values should I use for this line: #PBS -l select=1:ncpus=8:ompthreads=8
Will the job stop end when the script is

complete? Or do I need to add that into my script?

Cheers,

Derek Pierson

Request created
14/Oct/22 1:45 PM