Statistical and Mathematical Software on HPC systems

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Research Analytics
Plan of Attack

• Look at three packages on Big Red II: SAS, R, Matlab.
• Look at running a common task in all three.
• Discuss a bit on how the different packages take advantage of multicore or parallel functionality.
What modules am I using?

module load ccm
module load matlab
module load r
module load sas
module load cudatoolkit

For all these most recent version of the package is the default.
Three roads to parallelism

• Implicit parallelism (my favorite)
• Small modifications to existing code
• Fiddling around with mpi
SAS: background

• First developed in 1966 at North Carolina State for regression and analysis of variance.

• Commercialized in 1976 when the SAS Institute incorporates.

• Solid workhorse statistical package

• Still has not been used as a New York Times crossword clue, but both “Special Air Service” and “Scandinavian Airlines System” have.
SAS: starting it up

~> module load sas

SAS data analysis and management system version 9.4 loaded.

~> sas –nodms

More common to write the sas program and run it as a script

~> sas lineExample.sas

A SAS program has two steps: a data step and a proc step.
SAS: loading data and regressing

Look at the example of fitting a line through some data.

The csv file faithful.csv has 272 values.
We use SAS to find the line of best fit.
The file lineExample.sas

data faithful;
  infile "faithful.csv" delimiter="",";
  input x y;
run;

proc reg;
  model y = x;
run;
~>sas lineExample.sas

The output goes to lineExample.lst
SAS: loading data and regressing

~> tail -n 7 lineExample.lst

Parameter Estimates

| Parameter | Estimate  | Standard Error | t Value | Pr > |t| |
|-----------|-----------|----------------|---------|------|---|
| Intercept | 33.47440  | 1.15487        | 28.99   | <.0001 |
| x         | 10.72964  | 0.31475        | 34.09   | <.0001 |

Sure, $y = 10.72964 \times x + 33.47440$ seems okay.
SAS: producing graphics

Running canada.sas will save create an HTML file and a graphic in gchart.png

ods listing close;
ods html style=money
file="CanadaGraph.html";
proc gchart data=sashelp.prdsale;
vbar Product / sumvar=actual;
title1 "First Quarter Sales in Canada";
where Quarter=1 and Country="CANADA";
run;
quit;
ods html close;
ods listing;

~>sas canada.sas
SAS: implicit parallelism example

• SAS will create threads to run faster on multicore environments.
• This happens by default but we can see the improvement if we force SAS to run without threads.
• The next example involves taking the mean of a set of 50,000,000 random numbers.
### SAS: implicit parallelism example

%let NObs = 50000000;
data Unif(keep=u);
call streaminit(123);
do i = 1 to &NObs;
   u = rand("Uniform");  /* U[0,1] */
   output;
end;
run;

proc means data=unif;
var u;
run;

NOTE: PROCEDURE MEANS used
(Total process time):
   real time 1.76 seconds
   cpu time 4.37 seconds

%let NObs = 50000000;
data Unif(keep=u);
call streaminit(123);
do i = 1 to &NObs;
   u = rand("Uniform");  /* U[0,1] */
   output;
end;
run;

proc means data=unif;
var u;
run;

NOTE: PROCEDURE MEANS used
(Total process time):
   real time 3.63 seconds
   cpu time 3.57 seconds
R: background

• First created in the early 1990s by Ross Ihaka and Robert Gentleman as an implementation of S.

• Development soon shifted to a larger core group.

• Distributed under the GNU General Public License.
R: starting it up

`module load R`

`R`
The question mark will display a function’s help text. This is a shortcut for the `help()` function

```
help(sin)
? sin
```

The command `invisible()` suppresses output

The up arrow key will go back to previous commands

The command `system()` is used for shell commands

```
system("rm core")
```

The `rm()` command clears variables

```
rm(list=ls(all=TRUE)) #Clear all variables
```

The hash tag is used for comments

```
#This is an R comment
```
R: loading data and regressing

Let’s load the file faithful.csv again and rerun the earlier regression.

```r
faith <- read.csv("faithful.csv", header=FALSE)
faith
   V1 V2
1  3.600 79
2  1.800 54
lm(faith$V2 ~ faith$V1)
Call:
lm(formula = faith$V2 ~ faith$V1)
Coefficients:
(Intercept)    test2$V1
  33.47       10.73
```
R: plotting data

You don’t need an X11 connection to generate graphics

```r
fit<-lm(faith$V2~faith$V1)
png()
plot(faith$V1,faith$V2)
abline(fit$coefficients)
dev.off()
```

Default name is “Rplot001.png”.
R: multicore versions of apply()

R has many mapping functions that apply a function to the elements of a list, vector, what-have-you. The function lapply() applies a function to the elements of a list. The function mcapply() is a multicore version of lapply. The function rep(m,n) repeats m for n time. So lapply(rep(100,1000000),rnorm) returns 1000000 lists of 100 random numbers from a normal distribution.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>st&lt;-system.time(invisible(</td>
<td>library(parallel)</td>
</tr>
<tr>
<td>lapply(rep(100,1000000),</td>
<td>stm&lt;-system.time(invisible(</td>
</tr>
<tr>
<td>rnorm)))</td>
<td>mclapply(rep(100,1000000),</td>
</tr>
<tr>
<td>st[3]</td>
<td>rnorm,mc.cores=32))</td>
</tr>
<tr>
<td>elapsed 22.634</td>
<td>elapsed 4.066</td>
</tr>
</tbody>
</table>

The function rep(m,n) repeats m for n time. So lapply(rep(100,1000000),rnorm) returns 1000000 lists of 100 random numbers from a normal distribution.
Matlab: background

• Developed by Cleve Moler in the 1970s to give students easier access to numerical libraries for linear algebra (Matrix Laboratory)
• MathWorks company founded in 1984 for commercial development
• About 1900 IU network users 2013-14 academic year
• Decent support for parallelism
Matlab: starting it up

~> module load matlab
MATLAB numerical calculation framework version 2014a loaded.
~> matlab
Matlab: some useful tidbits

- The help command will display a function’s help text. The doc command brings up more information
  ```matlab
  help sin
  doc sin
  ```
- The semi-colon (;) will suppress output
- The up arrow key will go back to previous commands
- Typing and then using the up arrow key goes back to previous commands that start with that text
- The exclamation point is used for shell commands
  ```bash
  ! rm matlab_crash_dump.*
  ```
- The percent sign is used for comments
  ```matlab
  %This is a Matlab comment
  ```
Matlab: loading data and regressing

faith = csvread('faithful.csv');

x = faith(:,1);

y = faith(:,2);

fit = fitlm(x, y, 'linear')

Linear regression model:

\[ y \sim 1 + x_1 \]

Estimated Coefficients:

<table>
<thead>
<tr>
<th></th>
<th>Estimate</th>
<th>SE</th>
<th>tStat</th>
<th>pValue</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Intercept)</td>
<td>33.474</td>
<td>1.1549</td>
<td>28.985</td>
<td>7.136e-85</td>
</tr>
<tr>
<td>x1</td>
<td>10.73</td>
<td>0.31475</td>
<td>34.089</td>
<td>8.13e-100</td>
</tr>
</tbody>
</table>
Matlab: plotting data

```matlab
fit.plot
print( gcf,...
    '-dpng', 'MatlabPlot' )
```

This saves the plot as MatlabPlot.png.
Matlab: implicit parallelism in svd

Many functions will recognize that the multicore environment and create an appropriate number of threads.

Look at an example of two singular value decompositions. (Rewriting a matrix as the product of “nice” matrices.)
Matlab: implicit parallelism in svd

<table>
<thead>
<tr>
<th></th>
<th>&gt; matlab</th>
<th>&gt; matlab -singleCompThread</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>tic</td>
<td>tic</td>
</tr>
<tr>
<td></td>
<td>svd(rand(5000))</td>
<td>svd(rand(5000))</td>
</tr>
<tr>
<td></td>
<td>toc</td>
<td>toc</td>
</tr>
</tbody>
</table>

Elapsed time is 67.720321 seconds. Elapsed time is 157.032804 seconds.

Older versions of Matlab allowed you to set the maximum number of threads with `maxNumCompThreads`, but this is being deprecated.
Matlab: svd using the gpu

<table>
<thead>
<tr>
<th>qsub -l -q debug_gpu -lgres=ccm</th>
<th>qsub -l -q debug_gpu -lgres=ccm</th>
</tr>
</thead>
<tbody>
<tr>
<td>ccmlogin</td>
<td>ccmlogin</td>
</tr>
<tr>
<td>matlab</td>
<td>matlab</td>
</tr>
<tr>
<td>tic</td>
<td>tic</td>
</tr>
<tr>
<td>svd(rand(5000))</td>
<td>svd(rand(5000,'gpuArray'));</td>
</tr>
<tr>
<td>toc</td>
<td>toc</td>
</tr>
</tbody>
</table>

Elapsed time is 62.310409 seconds.  
Elapsed time is 16.616624 seconds.
Matlab: parallel-enabled functions

Many Matlab functions can use a pool of worker processes if you explicitly create them and tell the function to use them.

Sample problem: maximize the function $x_1^2 + 4\sin(5x_2)$ subject to the constraint $(x_1-1)^2 + (x_2-1)^2 = 25$

We first write a function to define the constraint mycon.m.

```matlab
function [c,ceq] = mycon(x)  
c = (x(1)-1)^2 + (x(2)-1)^2 - 25;  
ceq = [];```

Matlab: parallel-enabled functions

Then we set up the problem:

```matlab
opts = optimset('Algorithm','sqp');
problem = createOptimProblem('fmincon','objective', ...    @(x) x(1)^2 + 4*sin(5*x(2)),'x0',[3 3],'lb',[-5 -5], ...    'ub',[5 5],'nonlcon',@mycon,'options',opts);
ms = MultiStart;
```

The Matlab Multistart solver runs an optimizer from multiple start points. It’s natural to want to run it in parallel.

<table>
<thead>
<tr>
<th>ms.UseParallel = false; tic [x,f] = run(ms,problem,2000); toc</th>
<th>ms.UseParallel = true; tic [x,f] = run(ms,problem,2000); toc</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elapsed time is 48.502433 seconds.</td>
<td>Elapsed time is 4.673513 seconds.</td>
</tr>
</tbody>
</table>
Matlab: parallel-enabled functions

Matlab will more more than happy to let you run things in parallel even is it’s a really bad idea.

The optimizer patternsearch is an example. At each step patternsearch checks the values of the objective function at near the current point. The first point with a lower value becomes the current point for the next step.

You can, however, use a pool of workers and check them in parallel. This means checking all the nearby points.
Matlab: parallel-enabled functions

The code on the right is checking a full 1024 points at each step. Running it in parallel doesn’t make up for that.

| x0 = 0.4*ones(10,1); tic patternsearch(@(x)myFun(x,params), ... x0,[],[],[],[],0*x0,1+0*x0,[]); toc | parpool(32) options = psoptimset('UseParallel', true,... 'CompletePoll', 'on', 'Vectorized', 'off'); x0 = 0.4*ones(10,1); tic patternsearch(@(x)myFun(x,params), ... x0,[],[],[],[],0*x0,1+0*x0,[],options); toc delete(gcp) | Elapsed time is 0.476223 seconds. | Elapsed time is 4.673513 seconds. |
Matlab: parallel for loops

If you have a pool of parallel workers you use them to run a for-loop with parfor. The are some restrictions on the loop, but the main one is that the order of evaluation can’t matter. So the code below fails

```matlab
%Fibonacci failure
a(1)=1;a(2)=1;
parpool(2)
parfor i=3:100
    a(i)=a(i-1)+a(i-2);
end
delete(gcp)
```
Matlab: parallel for loops

An example that doesn’t fail

<table>
<thead>
<tr>
<th>tic for i=1:50000 a(i)=max(rand(100)); end toc</th>
<th>parpool(16) tic parfor i=1:50000 a(i)=max(rand(100)); end toc delete(gcp)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elapsed time is 11.202063 seconds.</td>
<td>Elapsed time is 2.629504 seconds.</td>
</tr>
</tbody>
</table>
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