

gputools: an R package for GPU computing

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GETTING UP AND RUNNING WITH gptools

- gptools is already installed on impact1.stat.iastate.edu, ready to load with `library(gptools)` in R.
- For other GPU systems, download gptools from CRAN with a simple `install.packages("gptools")` in R.
 - **WARNING:** installation will fail on non-GPU systems since the CUDA C compiler doesn't exist
- Documentation:
 - <http://brainarray.mbnl.med.umich.edu/Brainarray/Rgpgpu/>
 - <http://cran.r-project.org/web/packages/gptools/index.html>
 - <http://cran.r-project.org/web/packages/gptools/gptools.pdf>
- Requirements:
 - R (\geq version 2.8.0)
 - Nvidia's CUDA toolkit (\geq version 2.3)

CONTENTS OF gputools

A handful of selected R functions implemented with CUDA C for use on a GPU:

- Choose your device:

gputools function	CPU analog	Same usage?
chooseGpu()	none	NA
getGpuId()	none	NA

- Linear algebra:

gputools function	CPU analog	Same usage?
gpuDist()	dist()	no
gpuMatMult()	%*% operator	no
gpuCrossprod()	crossprod()	yes
gpuTcrossprod()	tcrossprod()	yes
gpuQr()	qr()	almost
gpuSolve()	solve()	no
gpuSvd()	svd()	almost

- Simple model fitting:

gputools function	CPU analog	Same exact usage?
gpuLm()	lm()	yes
gpuLsfit()	lsfit()	yes
gpuGlm()	glm()	yes
gpuGlm.fit()	glm.fit()	yes

- Hypothesis testing:

gputools function	CPU analog	Same exact usage?
gpuTtest()	t.test()	no

- Other useful algorithms:

gputools function	CPU analog	Same exact usage?
gpuHclust()	hclust()	no
gpuDistClust()	hclust(dist())	no
gpuFastICA()	fastICA() (fastICA package)	yes
gpuGranger()	grangertest() (lmtest package)	no
gpuMi()	???	???
gpuSvmPredict()	See www.jstatsoft.org/v15/i09/paper	no
gpuSvmTrain()	See www.jstatsoft.org/v15/i09/paper	no

MANAGING YOUR DEVICES: chooseGpu() AND getGpuId()

Background: Impact1 has four GPUs, each with a unique index from 0 to 3. To see this for yourself, log into impact1 and run the following:

```
[landau@impact1 ~]$ cd /usr/local/NVIDIA_GPU_Computing_SDK/C/bin/linux/release  
[landau@impact1 release]$ ./deviceQuery
```

Here are some pieces of the (quite verbose) output of `./deviceQuery`:

```
[deviceQuery] starting...
```

```
./deviceQuery Starting...
```

```
CUDA Device Query (Runtime API) version (CUDART static linking)
```

```
Found 4 CUDA Capable device(s)
```

```
Device 0: "Tesla M2070"
```

CUDA Driver Version / Runtime Version	4.1 / 4.1
CUDA Capability Major/Minor version number:	2.0
Total amount of global memory:	5375 MBytes (5636554752 bytes)
(14) Multiprocessors x (32) CUDA Cores/MP:	448 CUDA Cores
GPU Clock Speed:	1.15 GHz
Memory Clock rate:	1566.00 Mhz
Memory Bus Width:	384-bit
L2 Cache Size:	786432 bytes

Device 1: "Tesla M2070"

CUDA Driver Version / Runtime Version	4.1 / 4.1
CUDA Capability Major/Minor version number:	2.0
Total amount of global memory:	5375 MBytes (5636554752 bytes)
(14) Multiprocessors x (32) CUDA Cores/MP:	448 CUDA Cores
GPU Clock Speed:	1.15 GHz
Memory Clock rate:	1566.00 Mhz
Memory Bus Width:	384-bit
L2 Cache Size:	786432 bytes

Device 2: "Tesla M2070"

CUDA Driver Version / Runtime Version	4.1 / 4.1
CUDA Capability Major/Minor version number:	2.0
Total amount of global memory:	5375 MBytes (5636554752 bytes)
(14) Multiprocessors x (32) CUDA Cores/MP:	448 CUDA Cores
GPU Clock Speed:	1.15 GHz
Memory Clock rate:	1566.00 Mhz
Memory Bus Width:	384-bit
L2 Cache Size:	786432 bytes

Device 3: "Tesla M2070"	
CUDA Driver Version / Runtime Version	4.1 / 4.1
CUDA Capability Major/Minor version number:	2.0
Total amount of global memory:	5375 MBytes (5636554752 bytes)
(14) Multiprocessors x (32) CUDA Cores/MP:	448 CUDA Cores
GPU Clock Speed:	1.15 GHz
Memory Clock rate:	1566.00 Mhz
Memory Bus Width:	384-bit
L2 Cache Size:	786432 bytes

Things to note:

- Device 3 is a GPU
- “Tesla M2070” is the name of the model of the GPU.
- Device 3 contains multiple cores, or “sub-processors”.
From the output, it has 448 CUDA-capable cores.

EXAMPLE: MATRIX MULTIPLICATION

Now, suppose I want to do a giant matrix multiplication on Device 3. I'm automatically set to Device 0:

```
> getGpuId()
[1] 0
```

So I change to Device 3:

```
> chooseGpu(3)
[[1]]
[1] 3
```

and then if I want, I can verify the change:

```
> getGpuId()
[1] 3
```

Now, I define the matrices that I want to multiply on Device 3:

```
> A <- matrix(runif(1e+7), nrow = 1e+4)
> B <- matrix(runif(1e+7), ncol = 1e+4)
```

Then, I tell the device to multiply A and B using the GPU hardware:

```
> ptm <- proc.time(); C <- gpuMatMult(A, B); proc.time() - ptm  
    user  system elapsed  
 2.959   2.190   5.159
```

Compare the run time to that of the analogous CPU run on impact1:

```
> ptm <- proc.time(); D <- A %*% B; proc.time() - ptm  
    user  system elapsed  
116.389   0.166 116.503
```

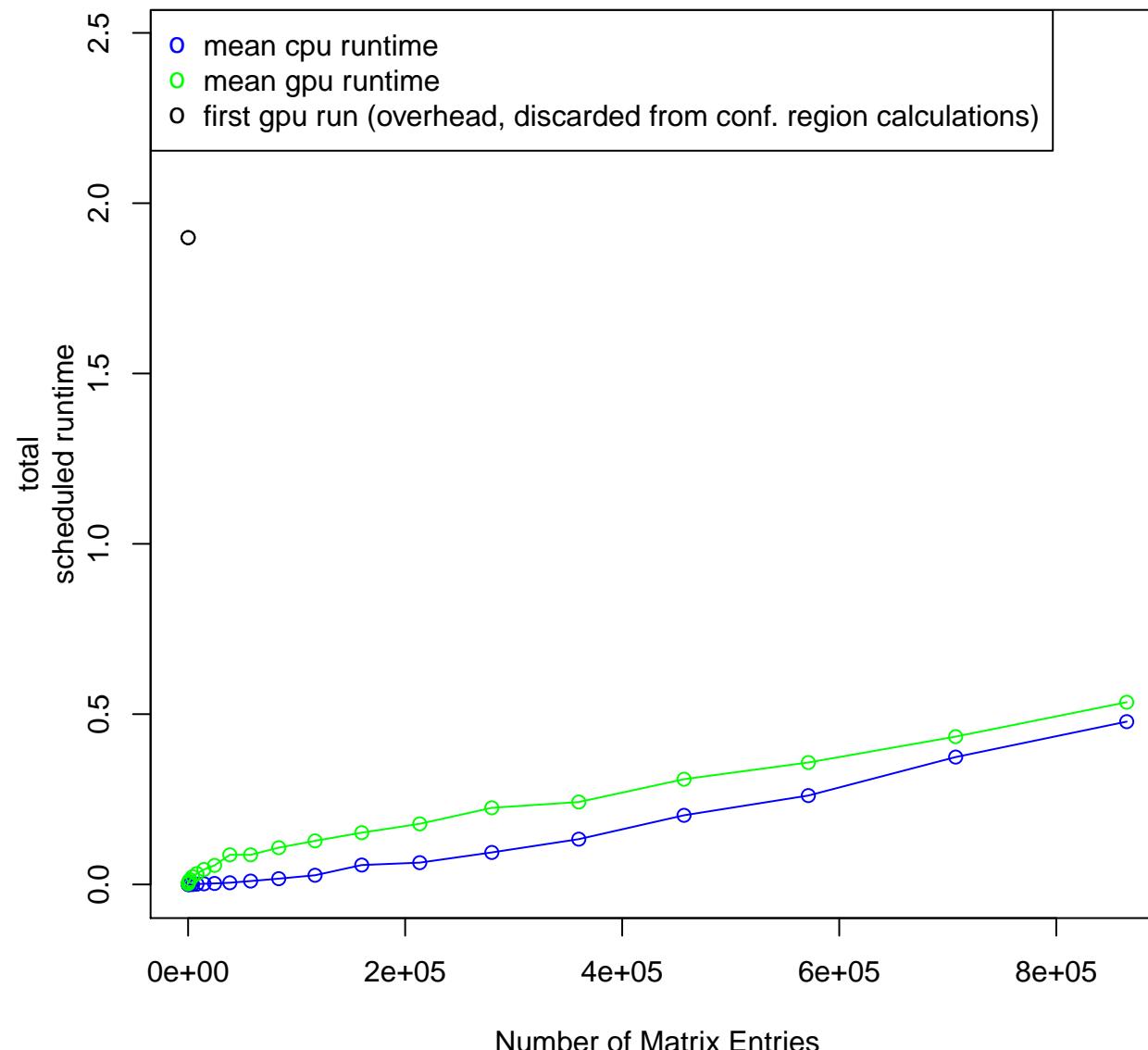
A COMPARISON OF `gpuQr()` AND `qr()`

The R script, `gpuQr.r`, compares the performance of `gpuQr(arg)` and `qr(arg)` for square matrices `arg` of varying sizes.

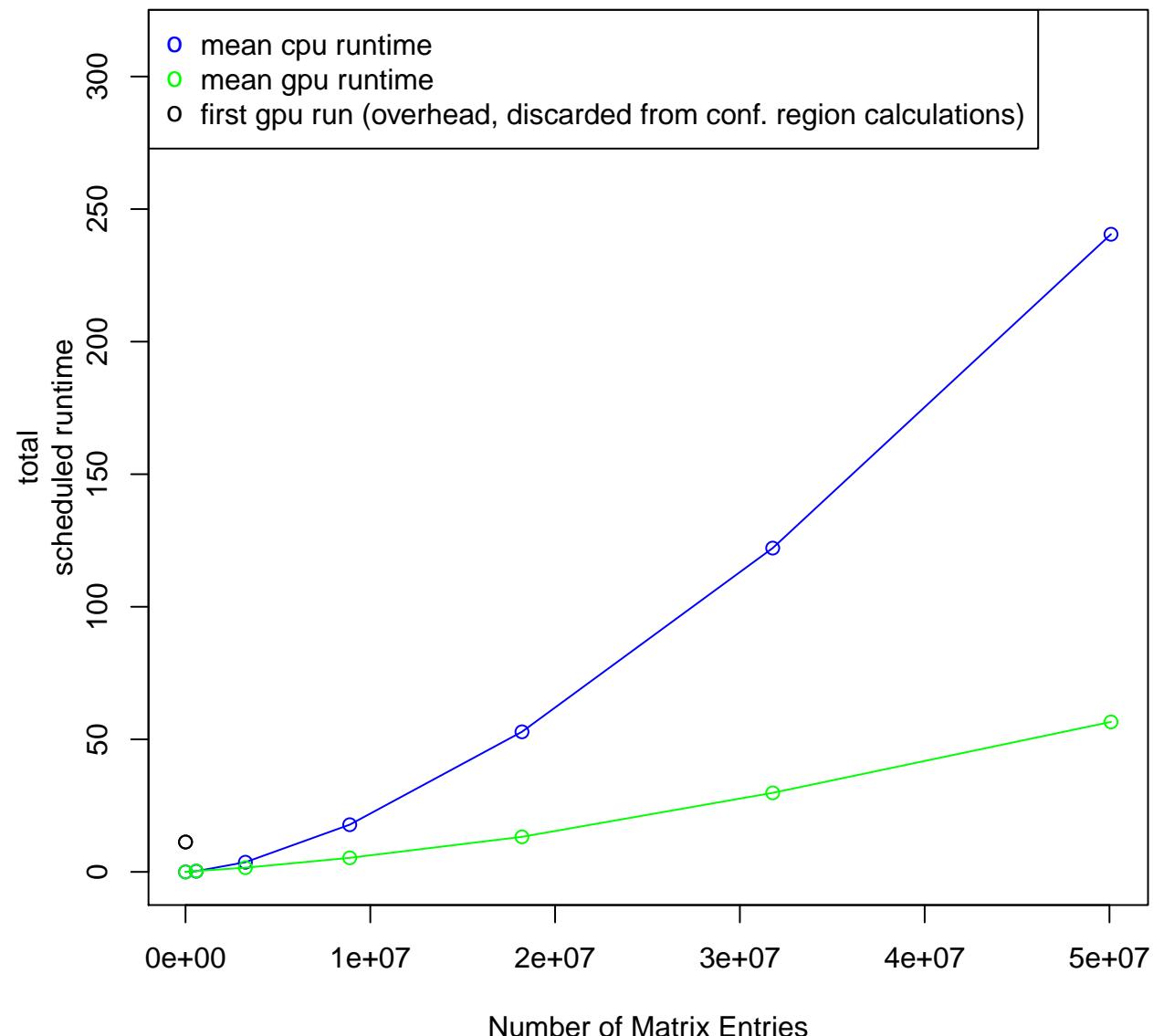
See the results on the next few slides.

NOTE: ALL TIMES ARE IN SECONDS.

**total
scheduled runtime:
 $qr()$ vs $gpuQr()$**



**total
scheduled runtime:
 $qr()$ vs $gpuQr()$**

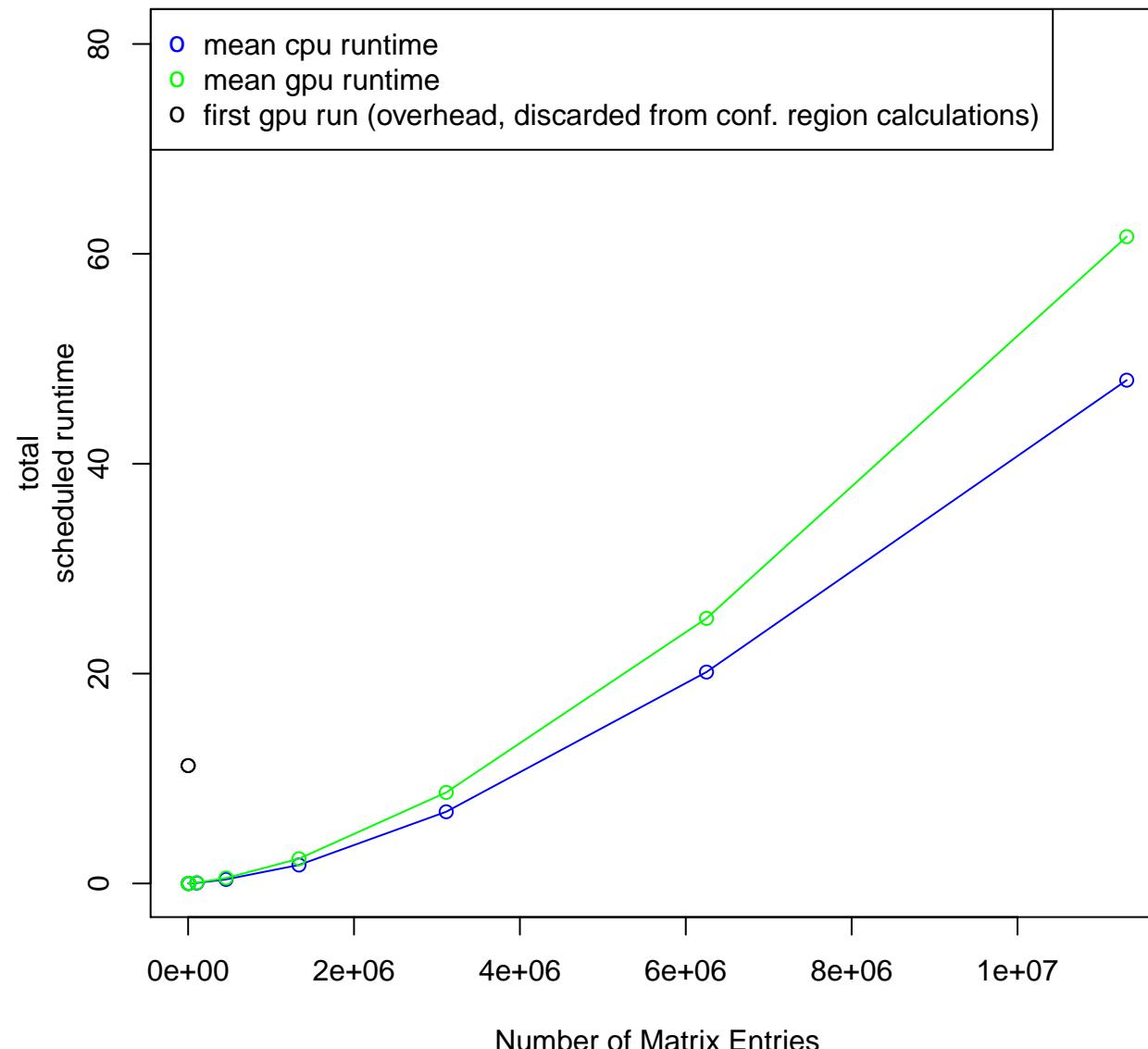


A COMPARISON OF `gpuSolve()` AND `solve()`

The R script, `gpuSolve.r`, compares the performance of `gpuSolve(arg)` and `solve(arg)` for square matrices `arg` of varying sizes.

See the results on the next few slides.

**total
scheduled runtime:
`solve()` vs `gpuSolve()`**

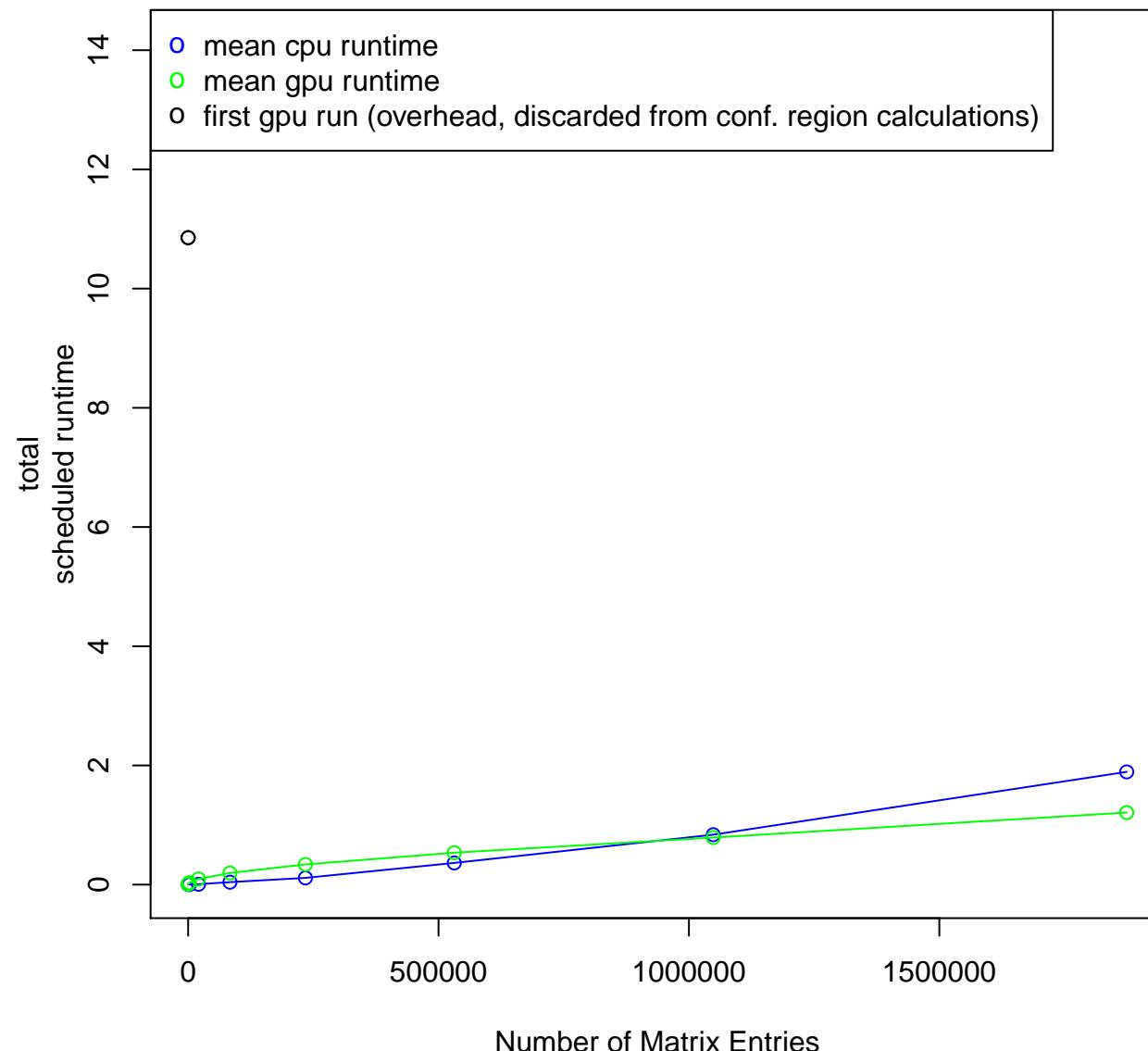


A COMPARISON OF `gpuLm()` AND `lm()`

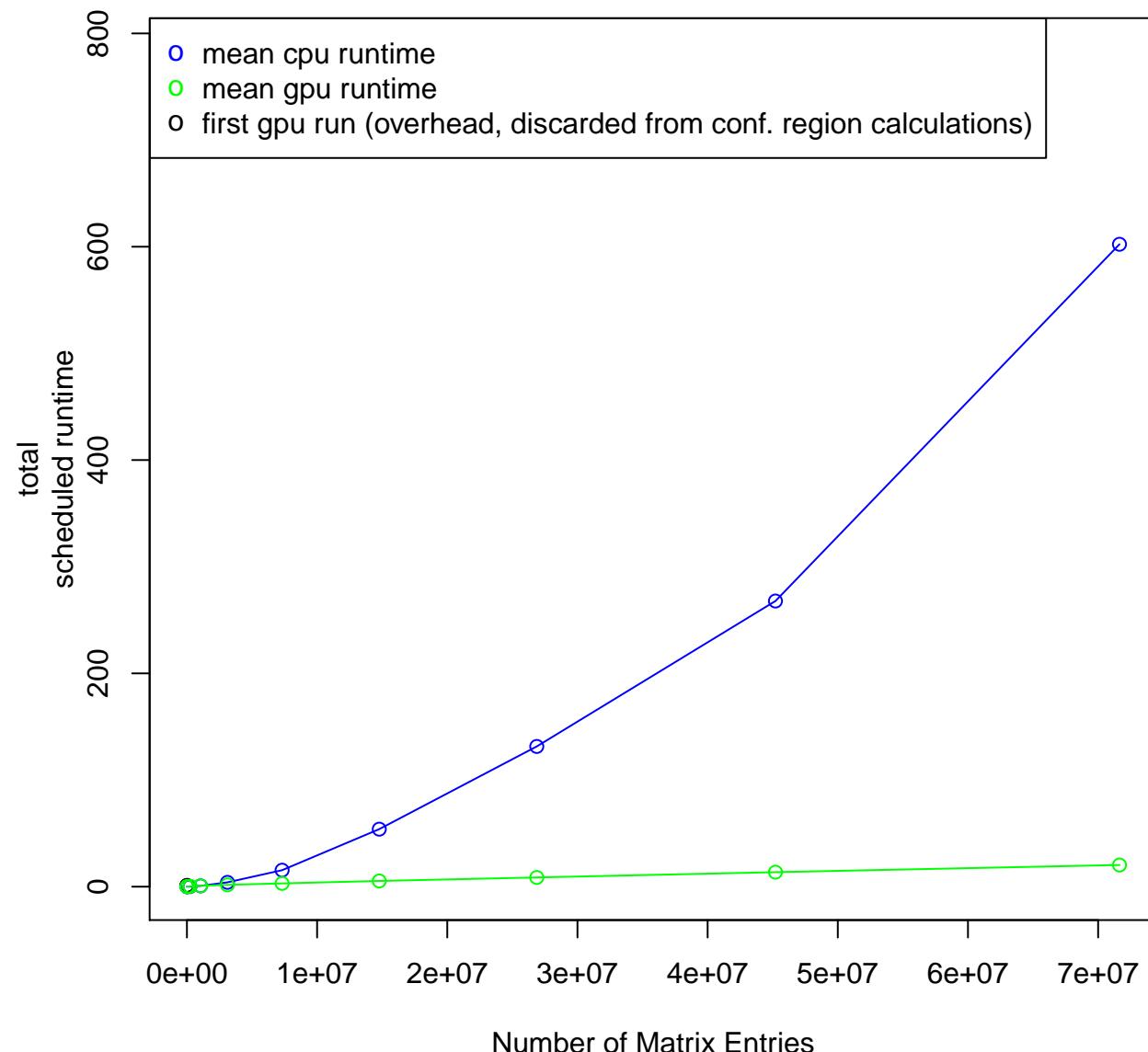
The R script, `gpuLm.r`, compares the performance of `gpuLm(y ~ x)` and `lm(y ~ x)` for matrices `y` and `x` of varying sizes.

See the results on the next slide.

**total
scheduled runtime:
 $\text{Im}()$ vs $\text{gpuLm}()$**



**total
scheduled runtime:
Im() vs gpuLm()**

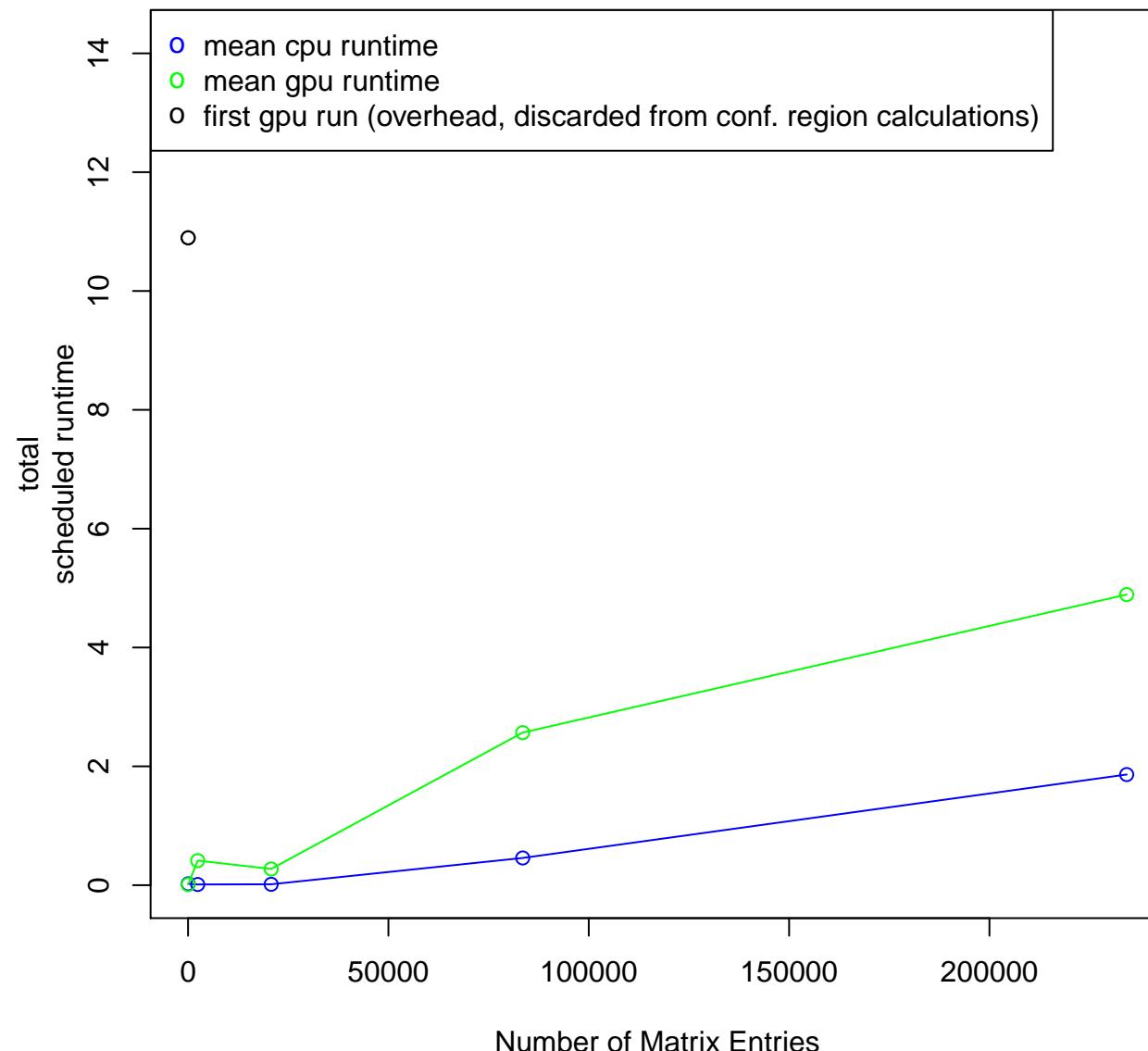


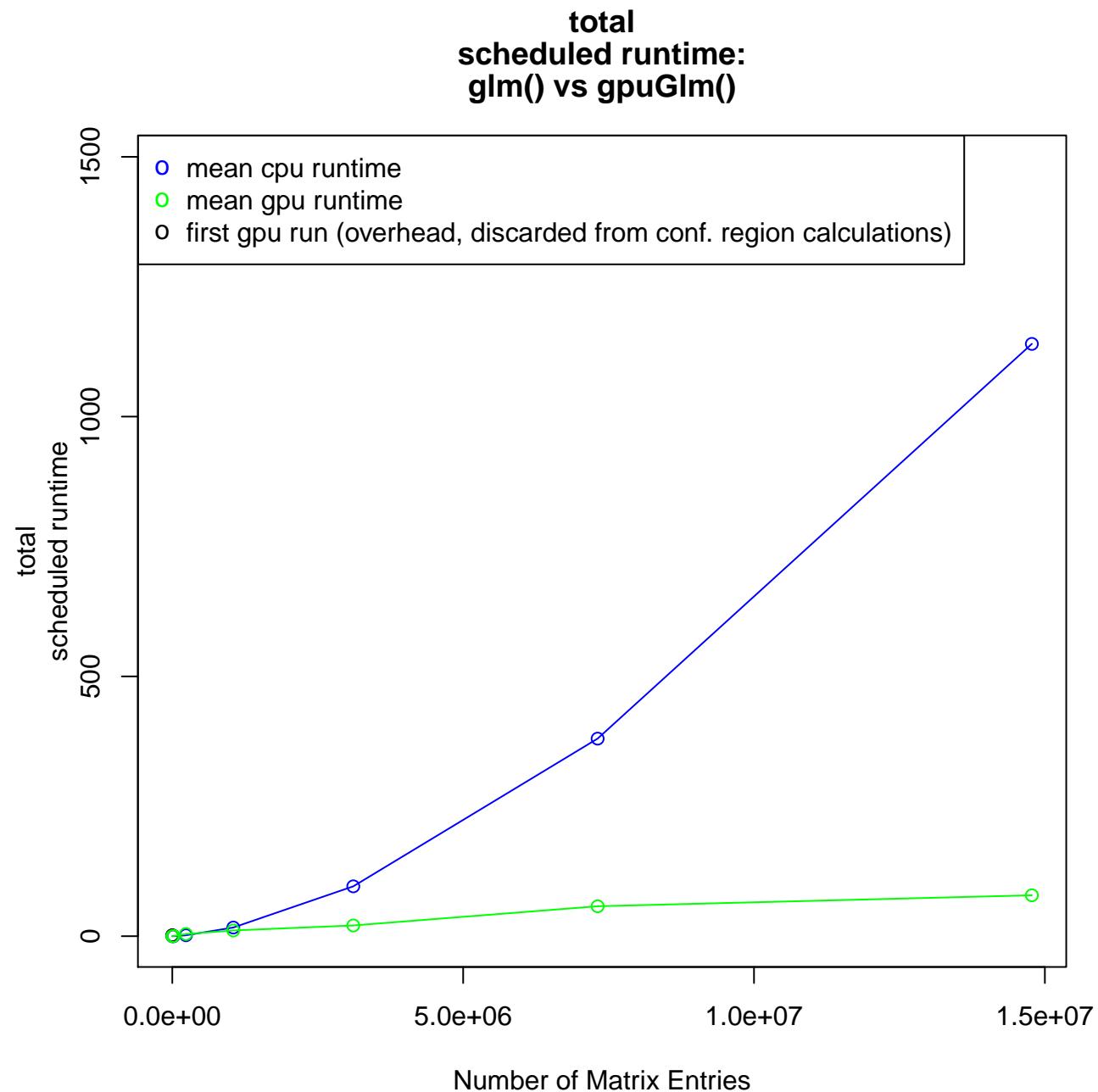
A COMPARISON OF `gpuGlm()` AND `glm()`

The R script, `gpuGlm.r`, compares the performance of `gpuGlm(y ~ x)` and `glm(y ~ x)` for matrices `y` and `x` of varying sizes.

See the results on the next few slides.

**total
scheduled runtime:
 $\text{glm}()$ vs $\text{gpuGlm}()$**





CLAIMS FROM THE AUTHORS OF gputools

(All of the following is from
<http://brainarray.mbnl.med.umich.edu/Brainarray/Rgpgpu/.>)

“Tested on a subset of GSE6306, non-GPU enabled fastICA took over four hours while gpuFastICA took just 80 seconds!”

Fig. 1: Speedup (R GPU vs. CPU)

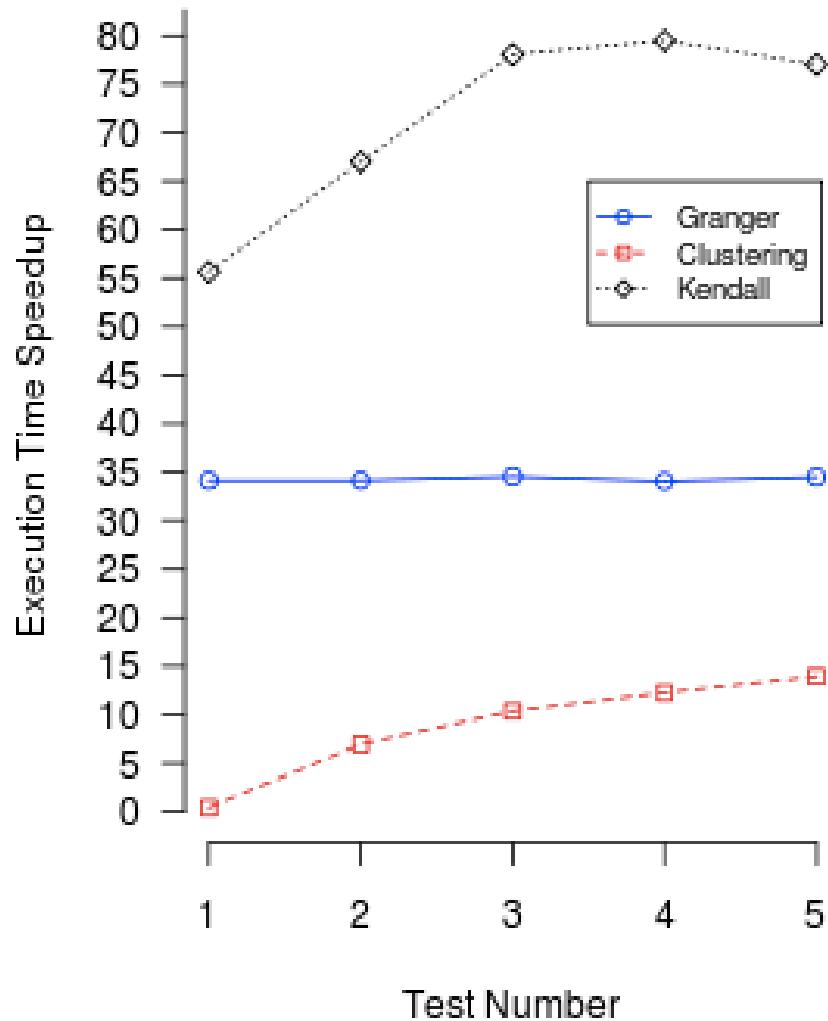


Fig. 2: Granger Times

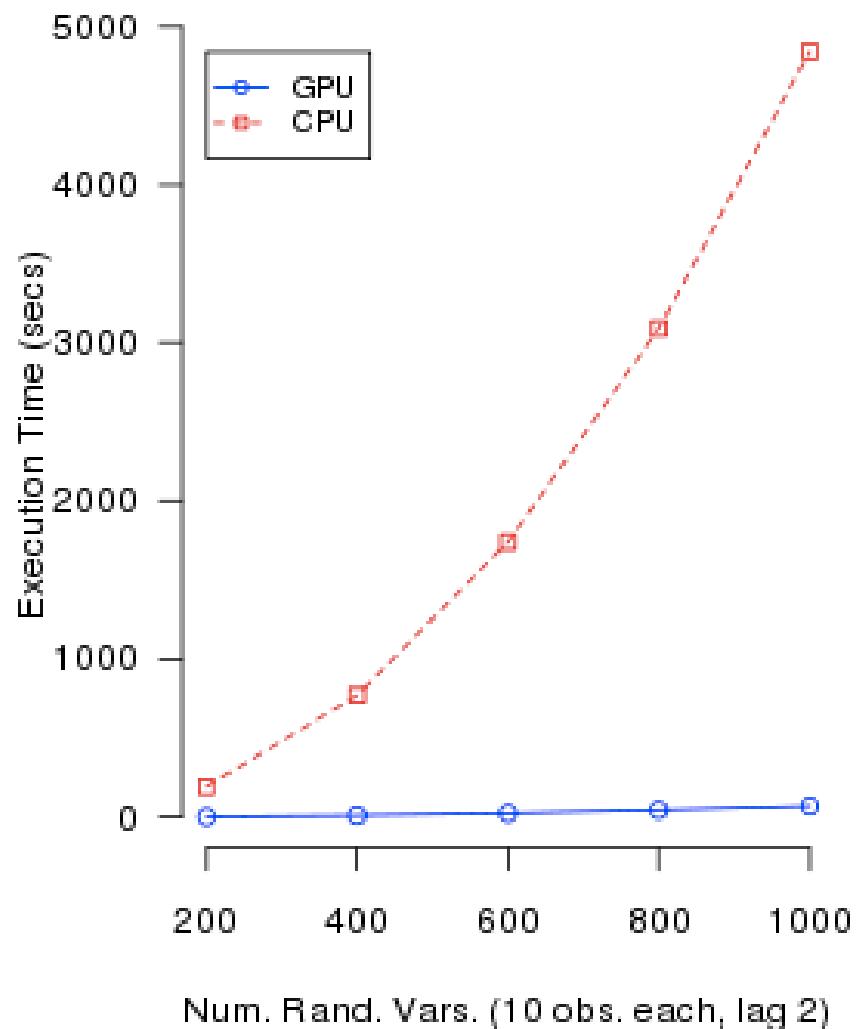


Fig. 3: Cluster Times

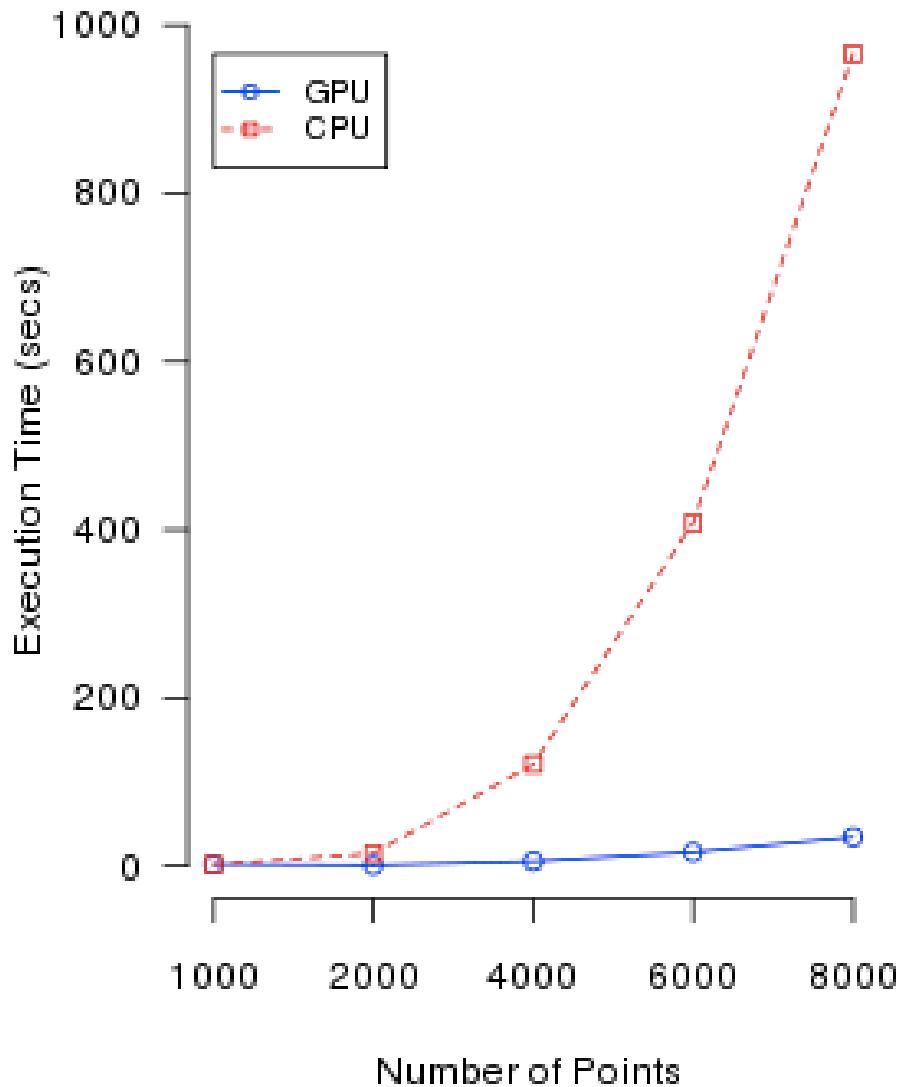
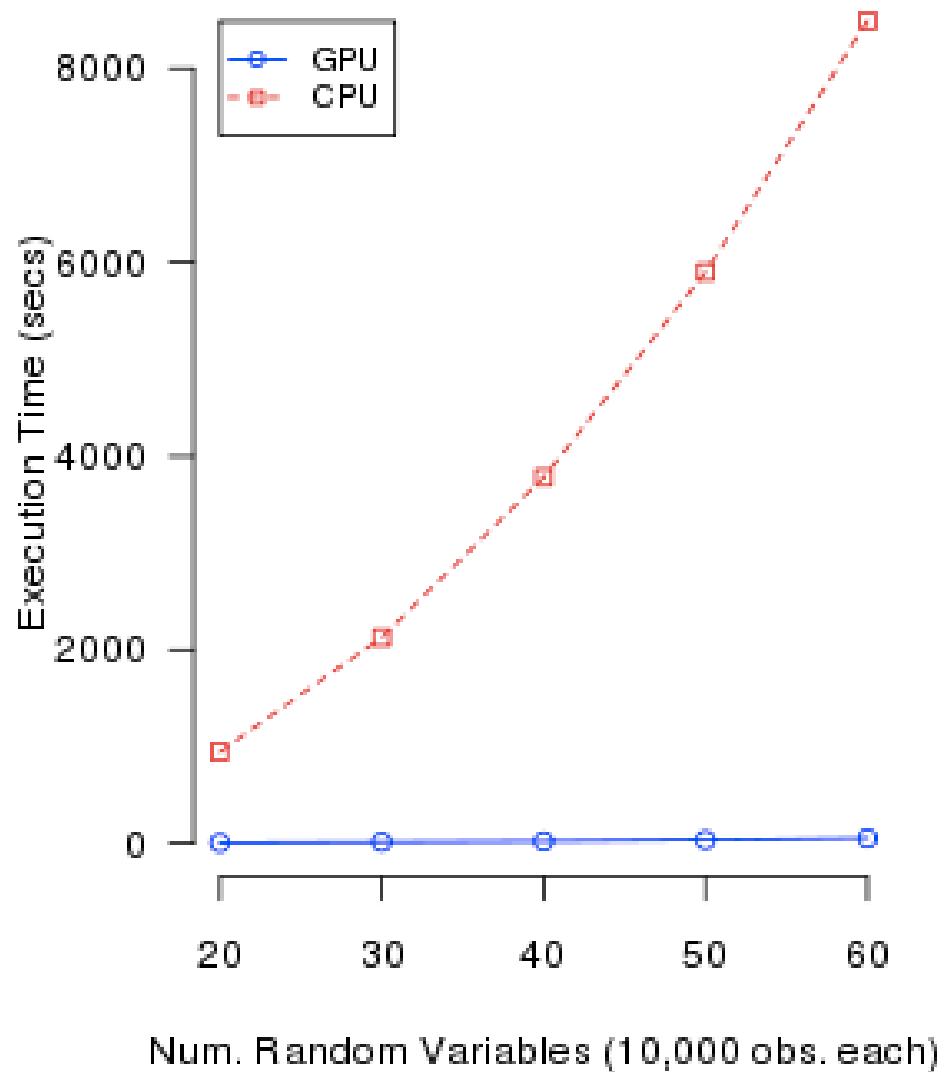


Fig. 4: Kendall Times



OTHER R PACKAGES FOR THE GPU

- WideLM - used to quickly fit a large number of linear models to a fixed design matrix and response vector.
- magma - a small linear algebra with implementations of backsolving and the LU factorization.
- cudaBayesreg - implements a Bayesian model for fitting fMRI data.
- gcbd - a Debian package for “benchmarking” linear algebra algorithms such as the QR, SVD and LU factorizations.

LECTURE SERIES MATERIALS

These lecture slides, a tentative syllabus for the whole lecture series, and code are available at:

<https://github.com/wlandau/gpu>.

After logging into you home directory on impact1, type:

```
git clone https://github.com/wlandau/gpu
```

into the command line to download all the course materials.

REFERENCES

- Josh Buckner, Mark Seligman, Justin Wilson. “R+GPU”.
<http://brainarray.mbnl.med.umich.edu/Brainarray/Rgpgpu/#introduction>.
- Dirk Eddelbuettel. “Package gcbd”.
<http://cran.r-project.org/web/packages/gcbd/gcbd.pdf>.
- Mark Seligman, Chris Fraley. “Package WideLM”.
<http://cran.r-project.org/web/packages/WideLM/WideLM.pdf>.
- Brian J Smith. “Package cudaBayesreg”.
<http://cran.r-project.org/web/packages/cudaBayesreg/cudaBayesreg.pdf>.