The Anatomy of a Science Engagement:

Analyzing the Human Connectome Project (HCP) Datasets using GPUs

John-Paul Robinson, MS Research Computing Day October 13, 2017

### Everything's going so well!!!



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12:48pm

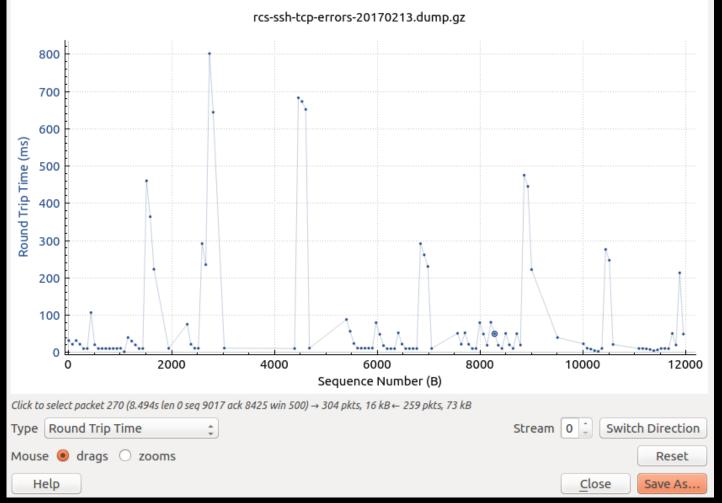
The viewer is lagging and freezing for extended periods. The connection has also been terminated during a session on several occasions this morning

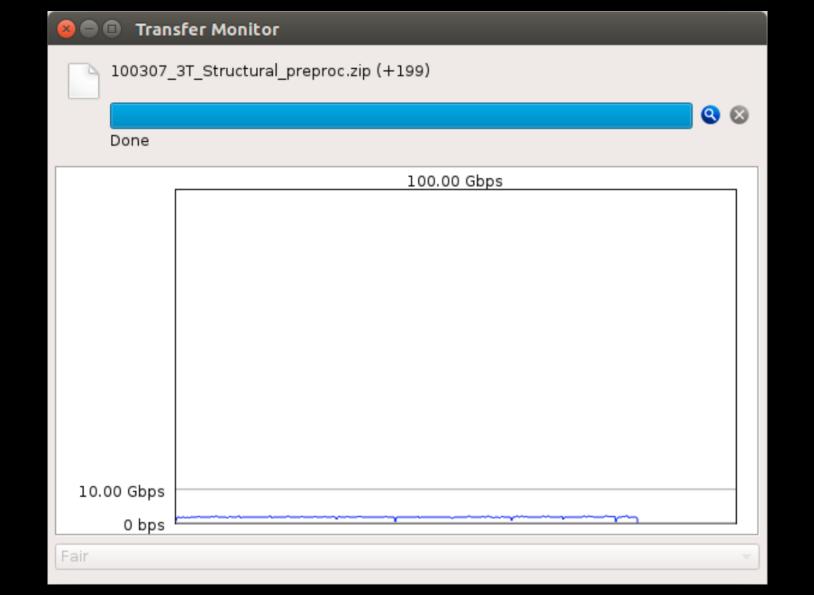
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# WTH!?!

#### Round Trip Time for 10.0.0.11:41794 → 164.111.161.5:22





### Impact of 1Gbps Data Flow

- Background:
  - UAB Campus Network and Firewall upgraded in Fall 2016
  - Campus now has 100Gbps to Internet and individual flows from off campus can reach multi-gigabit speeds
  - Campus core now has 40Gbps capacity
  - Traditional scp transfers only reach ~200Mbps flows and old campus board limited flows to 100's Mbps
  - Aspera Connect used by Human Connectome Project able to push 1.4Gbps flows
- Root cause:
  - Cluster network link to core needed upgrade from 1Gbps to 10G building speed
- New resources:
  - Science DMZ can transfer ~5 Terabytes per hour (so far...)

### Everything's going so well!!!



I am wanting to start an interactive job in cheaha, but cannot get past the "waiting for job to start" stage.

> Members of our lab are experiencing difficulty getting an S interactive terminal to load today.



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## Brainhack Global

March 2-5, 2017

#### **Toolkits for Brain Image Processing**



FSL is a comprehensive library of analysis tools for FMRI, MRI and DTI brain imaging data. It runs on Apple and PCs (both Linux, and Windows via a Virtual Machine), and is very easy to install. Most of the tools can be run both from the command line and as GUIs ("point-and-click" graphical user interfaces). – FSL docs

#### Bayesian Estimation of Diffusion Parameters Obtained using Sampling Techniques

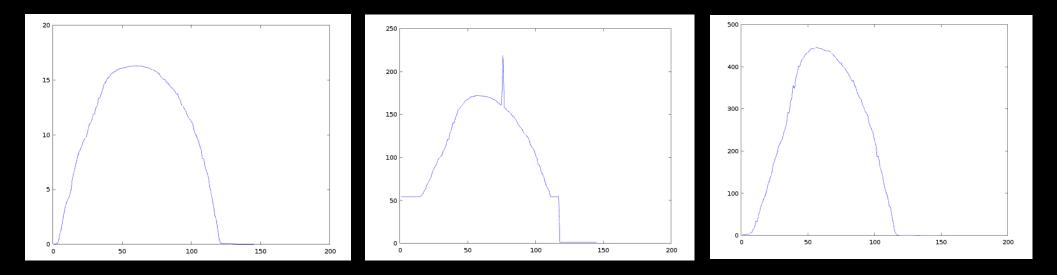
\varTheta 🔿 🔿 🔣 FDT – FMR	RB's Diffusion Too	olbox 2.0	
BEDPOSTX Estimation of diffusion parameters 🛁			
Input directory:			9
<ul> <li>✓ Advanced Options</li> <li>Fibres 2</li> <li>Weight 1</li> <li>Burn In 1000</li> <li>■ Multi-Shell model</li> <li>■ Model Noise Floor</li> <li>■ Rician Noise</li> </ul>			
Go	Exit	Help	

bedpostx allows to model crossing fibres within each voxel of the brain. Crucially, bedpostx allows to automatically determine the number of crossing fibres per voxel. – FSL docs

### What's Going On?

- Pre-processing HCP900 data set for Brainhack conference
  - 900+ subjects with over 1 TB of data to process
  - BEDPOSTX preps data and submits work to xfibres binary
- Problems
  - BedpostX scripts don't detect Slurm cluster, submit non-parallel jobs
  - Each subject consumes ~520 compute hours (21 days / single core)
  - Running all subjects at once uses 900 cores (40% cluster) but still takes 21 days
  - Cluster partition limits only apply per-job, not across multiple jobs
  - Cluster can flood with work from one user

#### **BEDPOSTX** is "Pleasantly Parallel"



File size per Slice (Megabytes)RAM per Slice (Megabytes)Tracks voxel count in sliceTracks voxel count in slice

**Runtime** per slice (Seconds) on singe core

#### What Did We Do?

- Understand BEDPOSTX operation
- Port BEDPOSTX scripts to recognize slurm and submit parallel jobs
- BEDPOSTX splits image into slices, about 145 slices/image
- Each slice runs in one job on single core
- Reduce processing time to 7 hours per subject
- Problems
  - Each subject consumes 145 cores or 6 cluster nodes
  - Could consume entire cluster for two weeks (16 days)

#### Enter the GPU



- CPUs use chip space for large, fast memory caches to speed execution of serial codes.
- GPUs use chip space to add 1000's of cores to speed execution of data-parallel codes

- Xfibres ported to GPU, 2013
- Cluster has 2x K80 GPUs with 2496 cores
- GPUs process one subject in 2 hours
- Still takes ~21 days to process whole data set because of limited GPU throughput (too few GPUs)
- CPUs are free for others

#### Lessons

- Use the cluster as you need to accomplish your science goals
- If performance is not what you expect, contact us. (And we may contact you! :) )
- Fixes are not always immediate
- Sometimes they involve a lot of work and lead to extended collaborations
- Maintaining software requires person hours all solutions shown here are still hand crafted and not in general code-base
- Need to grow software engineering practices for scientific computing

#### Outcomes

- Demonstrated reality of "Big Data" and advantages of GPU computing for select problems
  - Even if you can't use GPUs you should be happy your peers can!
  - GPUs help keep CPUs free for general purpose computing
- Contributed additional use-case to justify GPU expansion
- New GPUs can run BEDPOSTX on one HCP subject in 10
  minutes
- Entire HCP900 data set could now be run in 8.5 hours!
- Strengthened capability of UAB research and support teams

#### Keep doing what you do.

We promise we'll keep doing what we do.

# Special thanks to Kristina Visscher PhD, Sara Sims, and the Visual Brain Core