Cornell University
Center for Advanced Computing

Data Analysis with MATLAB

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MATLAB Has Many Capabilities for Data Analysis

- Preprocessing
  - Scaling and averaging
  - Interpolating and decimating
  - Clipping and thresholding
  - Extracting sections of data
  - Smoothing and filtering
- Applying numerical and mathematical operations
  - Correlation, basic statistics, and curve fitting
  - Fourier analysis and filtering
  - Matrix analysis
  - 1-D peak, valley, and zero finding
  - Differential equation solvers

Toolboxes for Advanced Analysis Methods

- Curve Fitting
- Filter design
- Statistics
- Communications
- Optimization
- Wavelets
- Spline
- Image processing
- Symbolic math
- Control system design
- Partial differential equations
- Neural networks
- Signal processing
- Fuzzy logic

Workflow for Data Analysis in MATLAB

- Access
  - Data files - in all kinds of formats
  - Software - by calling out to other languages/applications
  - Hardware - using the Data Acquisition Toolbox, e.g.
- *Pre-process… Analyze… Visualize…*
- Share
  - Reporting (MS Office, e.g.) - can do this with touch of a button
  - Documentation for the Web in HTML
  - Outputs for design
  - Deployment as a backend to a Web app
  - Deployment as a GUI app to be used within MATLAB

A Plethora of Routines for File-Based I/O

- High Level Routines
  - LOAD/SAVE
  - UIGETFILE/UIPUTFILE
  - UIIMPORT/IMPORTDATA
  - TEXTSCAN
  - XMLREAD/XMLWRITE
  - CSVREAD
  - DLMREAD/DLMWRITE
  - XLSREAD
  - IMREAD
- See “help iofun” for more
- Low Level Common Routines
  - FOPEN/FCLOSE
  - FSEEK/FREWIND
  - FTELL/FEOF
- Low Level ASCII Routines
  - FSCANF/FPRINTF
  - SSCANF/SPRINTF
  - FGETL/FGETS
- Low Level Binary Routines
  - FREAD/FWRITE

Example: Importing Data from a Spreadsheet

- Available functions: xlsread, dlmread, csvread
  - To see more options, use the “function browser button” that appears at the left margin of the command window
- Demo: Given beer data in a .xls file, use linear regression to deduce the calorie content per gram for both carbohydrates and alcohol

```
[num,txt,raw] = xlsread('BeerCalories.xls')
y = num(:,1)
x1 = num(:,2)
x2 = num(:,4)
m = regress(y,[x1 x2])
plot([x1 x2]*m,y)
hold on
plot(y,y,'r')
```

Share Results

- Push the “publish” button to create html, doc, etc. from a .m file
  - Feature has been around 5 years or so
  - Plots become embedded as graphics
  - Section headings are taken from cell headings
- Use cells to organize your work
  - Create cells in .m file by typing a %% comment
  - Cells can be re-run one at a time in the execution window if desired
  - Cells can be “folded” or collapsed so that just the top comment appears
- Share the code in the form of a deployable application
  - Simplest: send MATLAB code (.m file, say) to colleagues
  - Use MATLAB compiler to create stand-alone exes or dlls
  - Use a compiler add-on to create software components for Java, .NET

Lab: Setting Data Thresholds in MATLAB

- Look over count_nicedays.m in the lab files
  - Type “help command” to learn about any command you don’t know
  - By default, “dlmread” assumes spaces are the delimiters
  - Note, the “find” command does thresholding based on two conditions
  - Here, the .* operator (element-by-element multiplication) is doing the job of a logical “AND”
  - Try calling this function in Matlab, supplying a valid year as argument

- Exercises
  - Let’s say you love hot weather: change the threshold to be 90 or above
  - Set a nicedays criterion involving the *low* temps found in column 3
  - Add a line to the function so it calls “hist” and displays a histogram

The Function count_nicedays

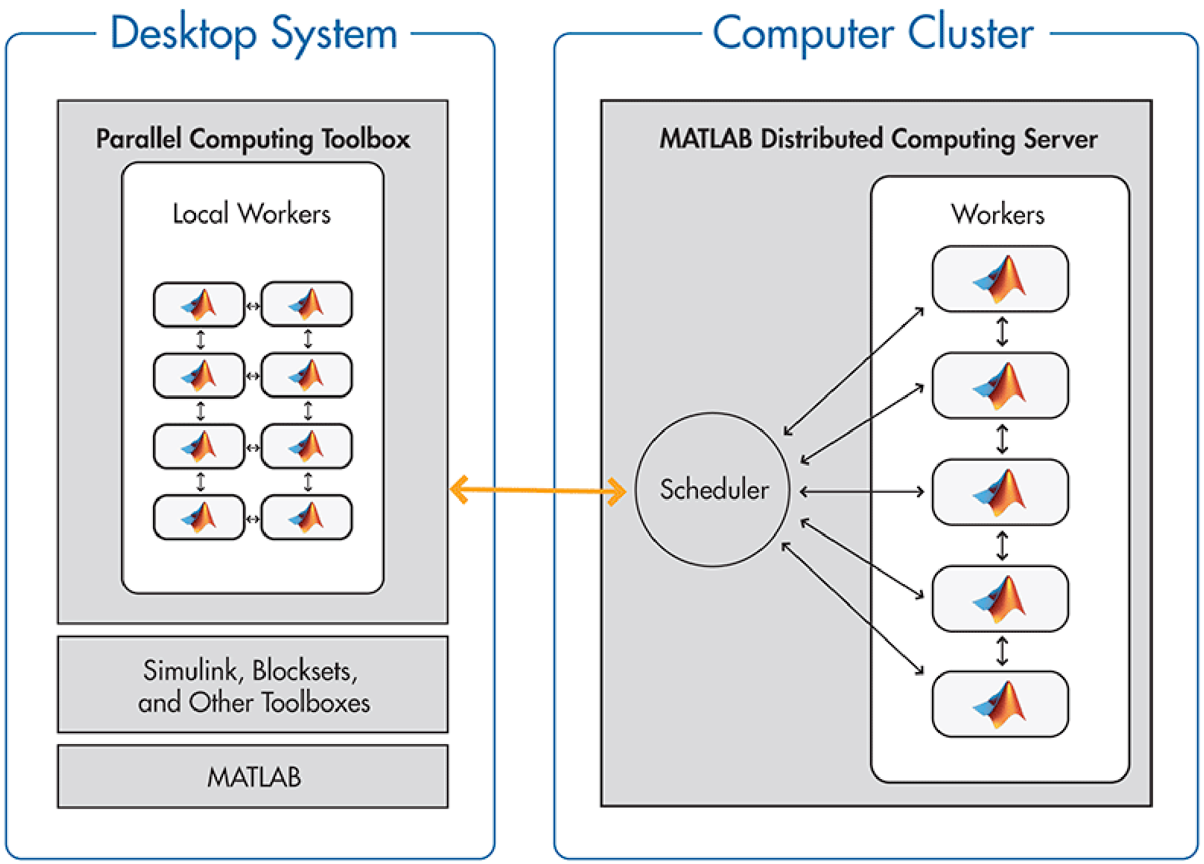
```
function nicedays = count_nicedays( yr )
%COUNT_NICEDAYS returns number of days with a high between 70 and 79.
%   It assumes data for the given year are found in a specific file
%   that has been scraped from the Ithaca Climate Page at the NRCC.

% validateattributes does simple error checking –
% e.g., are we getting the right datatype
validateattributes(yr,{'numeric'},{'scalar','integer'})
filenm = sprintf('ith%dclimate.txt',yr);
result = dlmread(filenm);
indexes = find((result(:,2)>69) .* (result(:,2)<80));
nicedays = size(indexes,1);

end
```

- What if we wanted to compute several different years in parallel?...

How to Do Parallel Computing in MATLAB

- Core MATLAB already implements multithreading in its BLAS and in its element-wise operations
- Beyond this, the user needs to make changes in code to realize different types of parallelism, in order of increasing complexity:
  - Parallel for loops (parfor)
  - Codistributed arrays, for big-data parallelism
  - Parallel code constructs and algorithms in the style of MPI
- The user’s configuration file determines where the workers run
  - Parallel Computing Toolbox - take advantage of multicores, up to 8
  - Distributed Computing Server - use computer cluster (or local cores)

Access to Local and Remote Parallel Processing



Dividing up a Loop Among Processors

```
for i=1:3
count_nicedays(2005+i)
end
```

- Try the above, then try this easy way to spread the loop across multiple processors (note, though, the startup cost can be high):

```
matlabpool
parfor i=1:3
count_nicedays(2005+i)
end
```

- Note, matlabpool starts extra copies of matlab.exe which do not count against the license; the size of this worker pool is set by the default “local” configuration - usually it’s 2 or 4, but it can go up to 8

What is *parfor* Good for?

- It can be used for *data parallelism*, where each thread works on independent subsections of a matrix or array
- It can be used for certain kinds of *task parallelism*, e.g., by doing a parameter sweep, as in our example (“parameter parallelism?”)
- Either way, all loop iterations must be totally independent
  - Totally independent = “embarrassingly parallel”
- Mlint will tell you if a particular loop can't be parallelized

- Parfor is exactly analogous to “parallel for” in OpenMP
  - In OpenMP parlance, the scheduling is “guided” as opposed to static
  - This means N threads receive many chunks of decreasing size to work on, instead of simply N equal-size chunks (for better load balance)

How to Do Nearly the Same Thing Without PCT

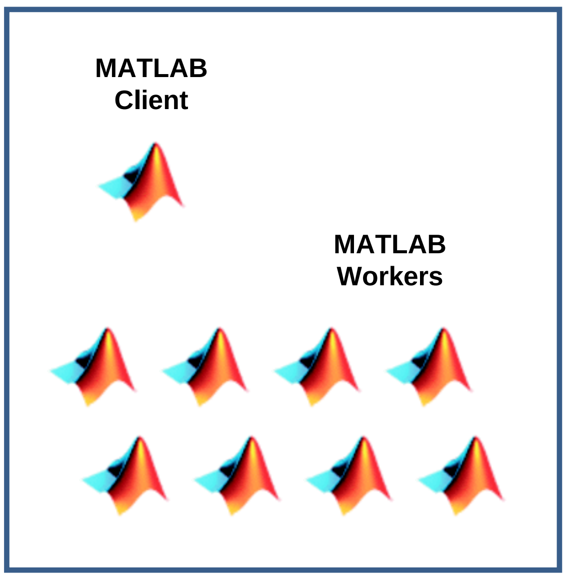
- Create a MATLAB .m file that takes one or more input parameters
  - The parameter may be the name of an input file, e.g.
- Use the MATLAB C/C++ compiler (mcc) to convert the script to a standalone executable
- Run N copies of the executable on an N-core machine, each with a different input parameter
  - In Windows, this can be done with “start /b”
- For fancier process control or progress monitoring, use a scripting language like Python
- This technique can even be extended to a cluster
  - mpirun can be used for remote initiation of non-MPI processes
  - The Matlab runtimes (dll’s) must be available on all cluster machines

Advanced Parallel Data Analysis

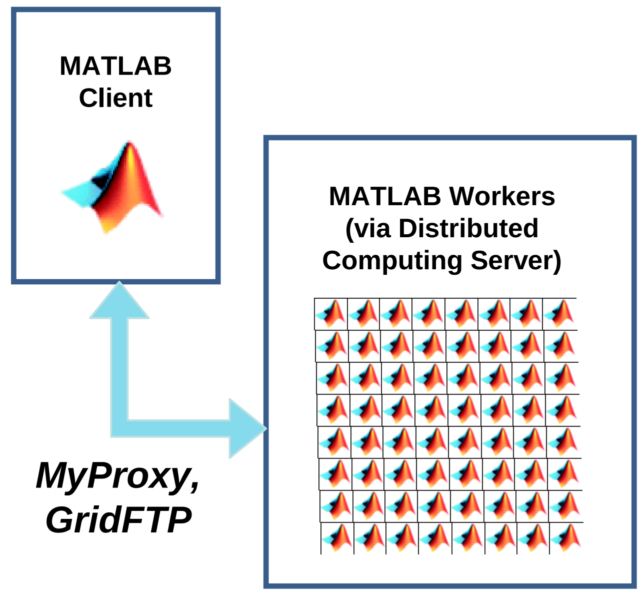
- Over 150 MATLAB functions are overloaded for codistributed arrays
  - Such arrays are actually split among mutliple MATLAB workers
  - In the command window, just type the usual e = d*c;
  - Under the covers, the matrix multiply is executed in parallel using MPI
  - Some variables are cluster variables, while some are local
- Useful for large-data problems that require distributed computation
  - How do we define large? - 3 square matrices of rank 9500 > 2 GB
- Nontrivial task parallelism or MPI-style algorithms can be expressed
  - createTask(job...), submit(job) for parallel tasks
  - Many MPI functions have been given MATLAB bindings, e.g., labSendReceive, labBroadcast; these work on all datatypes

New Way to Use the MATLAB PCT

CAC's client software extends the Parallel Computing Toolbox!



Select the local scheduler – code runs on client CPUs



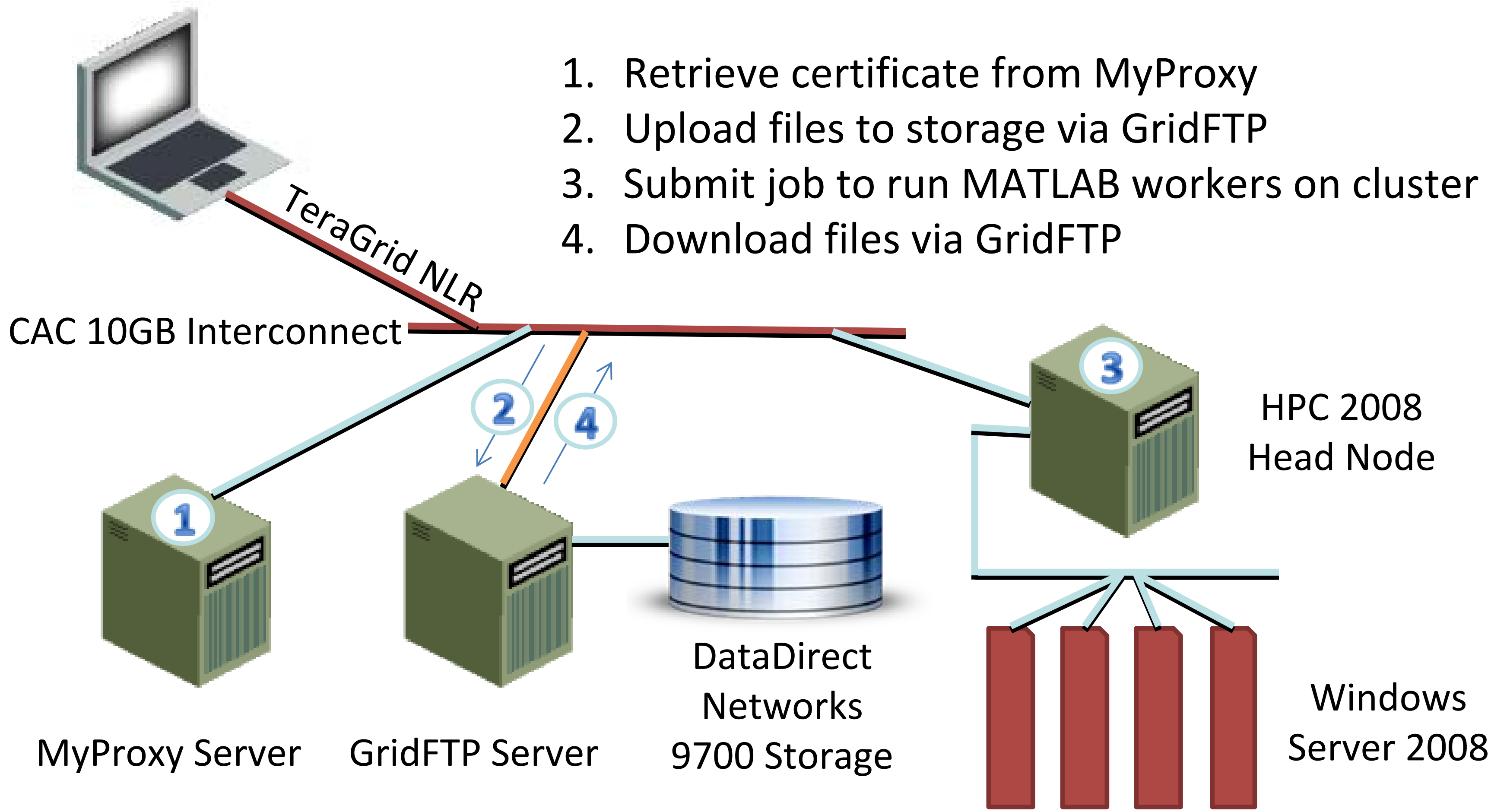
Select the CAC scheduler – Code runs on remote CPUs

Essential Services and Security

- File transfer service
  - Move files through a GridFTP (specialized FTP) server to a network file system that is mounted on all compute nodes
- Job submission service
  - Submit and query jobs on the cluster (via TLS/SSL); these jobs are to be executed by MATLAB workers on the compute nodes
- Security and credentials
  - Send username/password over a TLS encrypted channel to MyProxy; receive in exchange a short-lived X.509 certificate that grants access to the services

Hardware View

1. Retrieve certificate from MyProxy
2. Upload files to storage via GridFTP
3. Submit job to run MATLAB workers on cluster
4. Download files via GridFTP



System Specifications at CAC

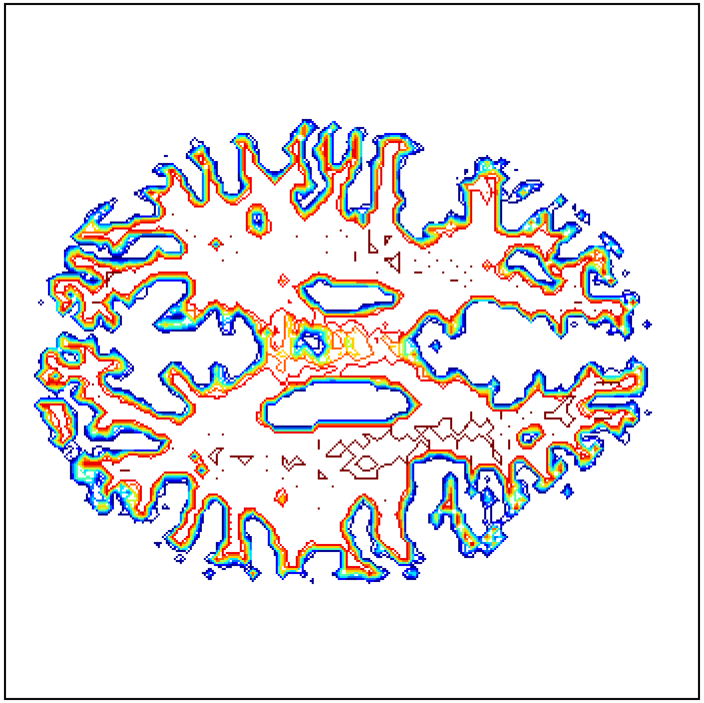
- Microsoft Windows HPC Server 2008 cluster
  - Supports MATLAB clients on Windows, Mac, and Linux
- 64 Dell™ PowerEdge™ M600 blade servers
  - 2 quad-core Intel® Xeon®/blade server, 512 total cores
  - 16GB RAM/blade server, 1TB total RAM
- 8TB DataDirect Networks storage
  - RAID-6 with on-the-fly read/write error correction
  - Accessible by all blade servers
  - Accessible externally via GridFTP
  - 10 Gb/s connectivity to TeraGrid
- Experimental hardware resource funded by NSF
  - Anyone can request an account via http://www.cac.cornell.edu/matlab

Example: Analysis of MRI Brain Scans

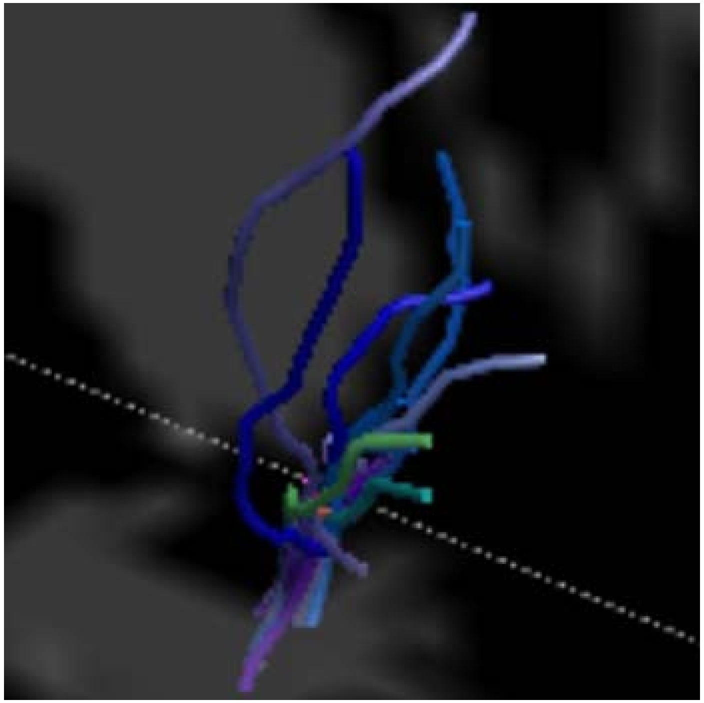
- Work by Ashish Raj and Miloš Ivković, Weill-Cornell Medical College
- Research question: Given two different regions of the human brain, how interconnected are they?
- Potential impact of this technology:
  - Study of normal brain function
  - Understanding medical conditions that damage brain connections, such as multiple sclerosis, Alzheimer’s disease, traumatic brain injury
  - Surgical planning

Connecting Two Types of MRI Data

- 3D MRI scans to map the brain's white matter

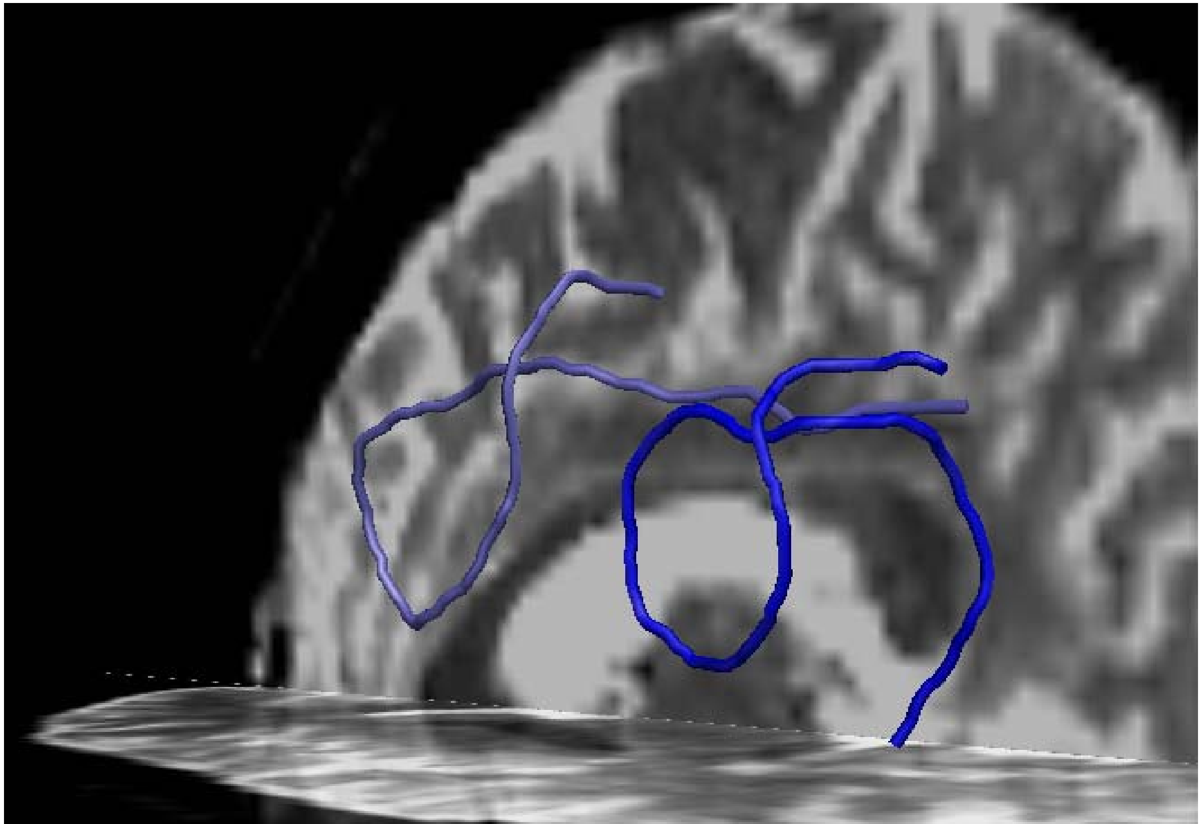


- Fiber tracts to show lines of preferential diffusion



Need for Computational Power

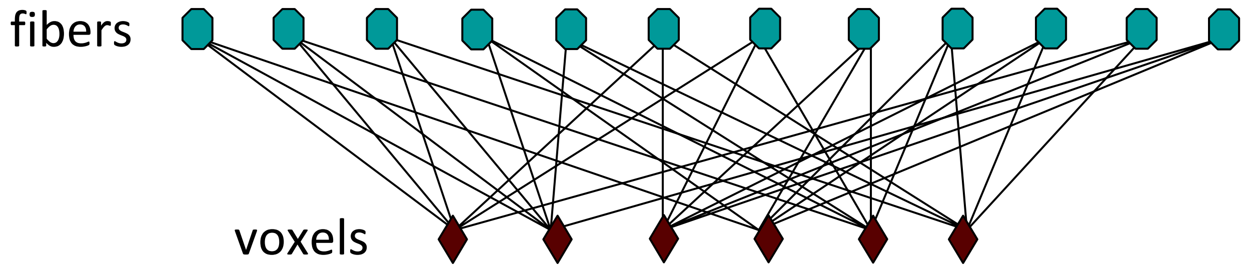
- Problem: long, spurious fibers arise in first-pass analysis
- Solution: use MATLAB to re-weight fibers according to importance in connections



Examples of improbable fibers eliminated by analysis

Connections in a Bipartite Graph

- Ivković and Raj (2010) developed a message-passing optimization procedure to solve the weighting problem
- Operates on a bipartite graph: nodes = fibers + voxels, edge weights = connection strength

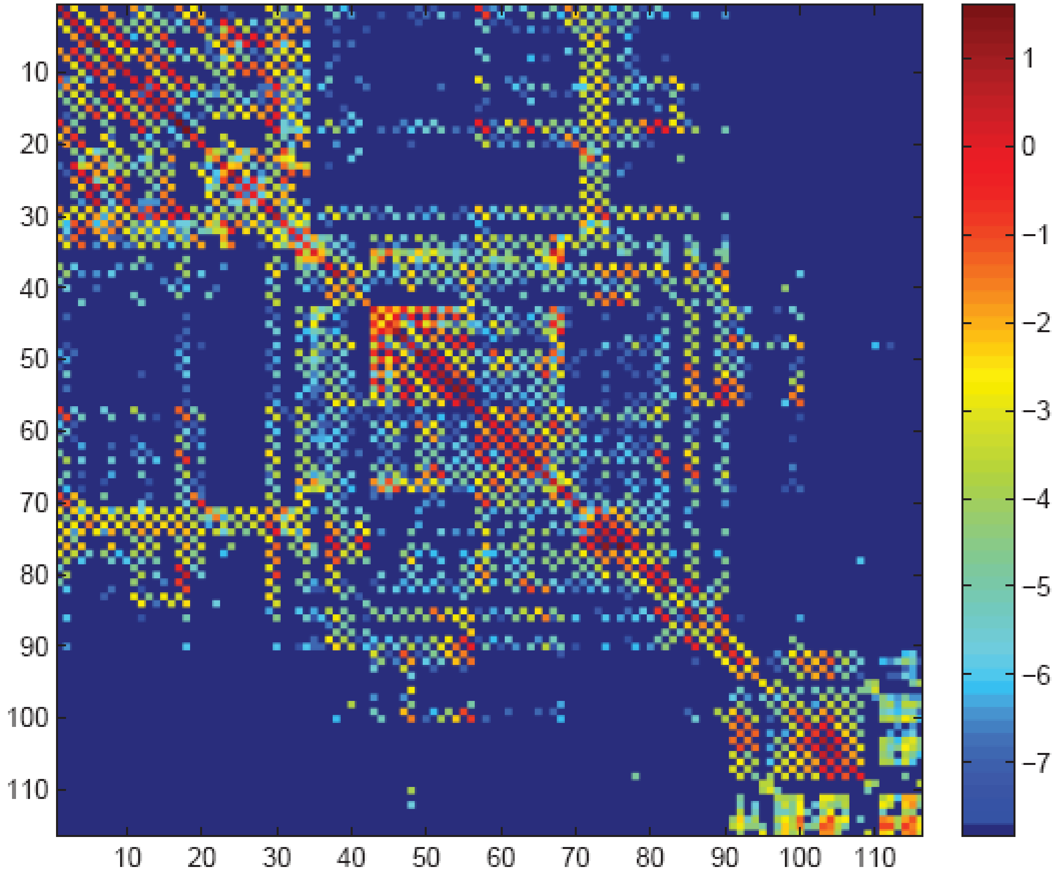


- MATLAB computations at each voxel are independent of all other voxels, likewise for fibers; *inherently parallel*
- Implementation with parfor in inner loop: 20x speedup on 8 cores

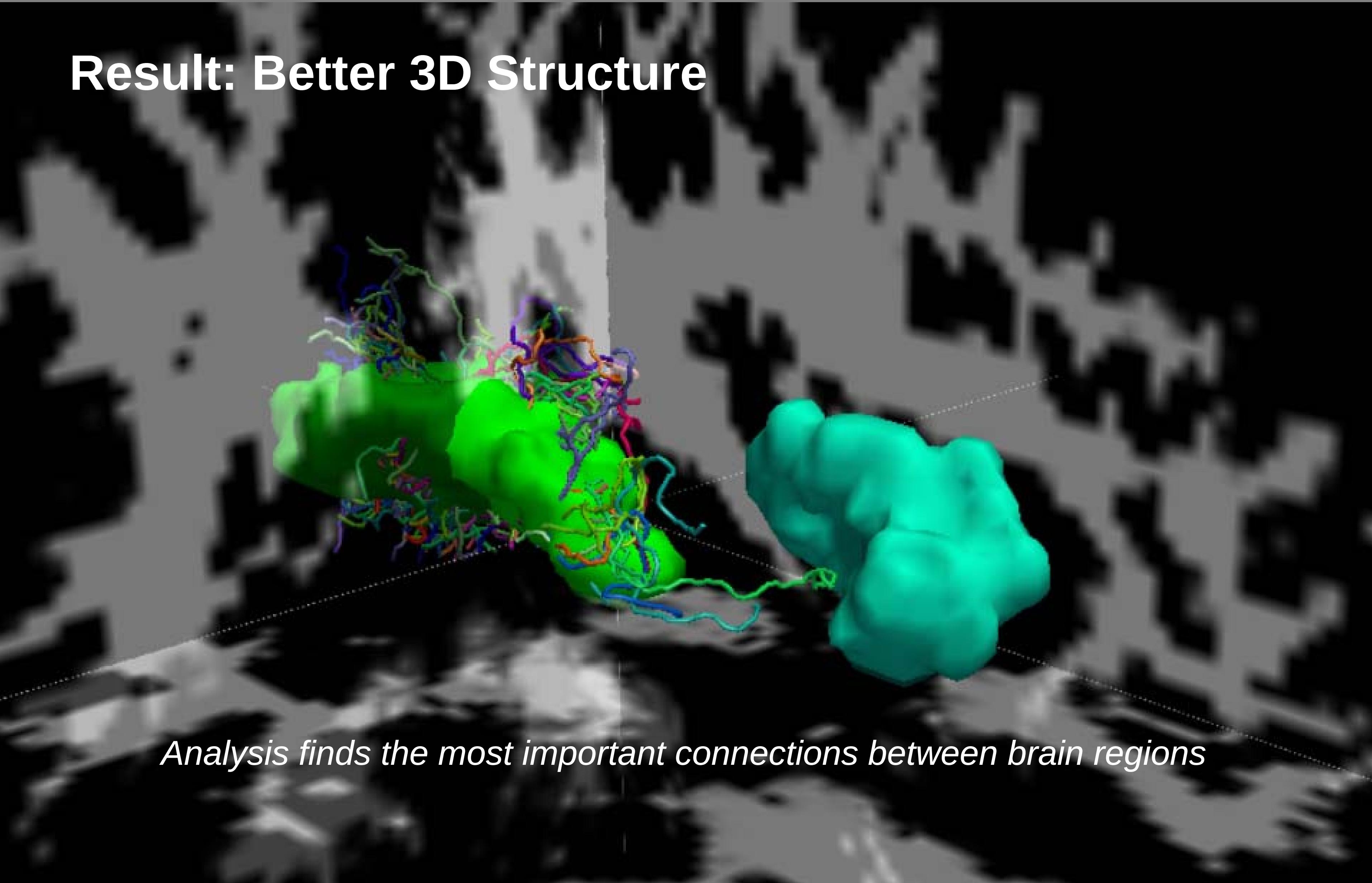
Data Product: Connectivity Matrix

- Graph with 360K nodes, 1.8M edges, optimized in 1K iterations

- The reduced digraph at right is based on 116 regions of interest



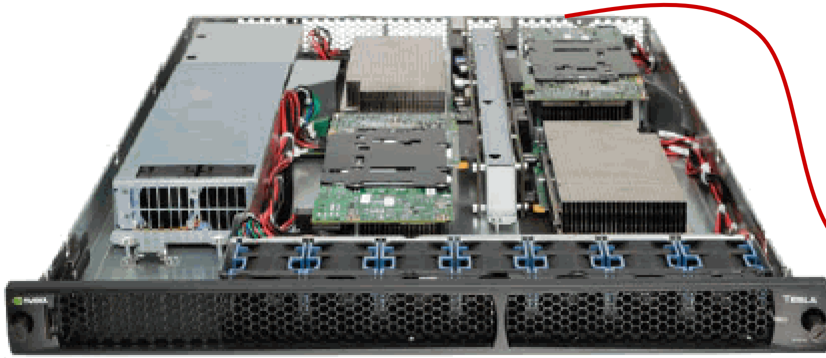
Result: Better 3D Structure



Analysis finds the most important connections between brain regions

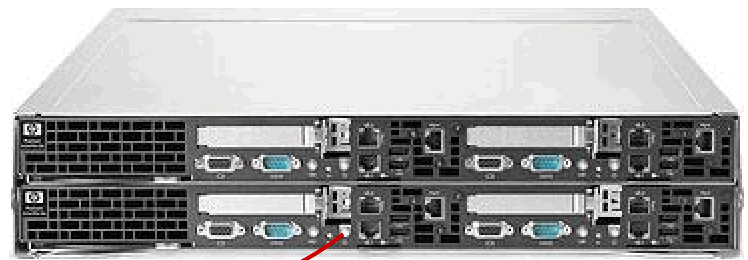
MATLAB GPU Computing Tests

NVIDIA Tesla S1070



Tested 1/4 T10 @ 1.44 GHz, 4 GB GDDR3; peak Tflop/s = 1.0 single, 0.1 double

HP ProLiant SL2x170z G6



Tested 1/4 server, 8/8 cores, Nehalem-EP @ 2.93 GHz, 24 GB DDR3; peak Tflop/s = 0.2 single, 0.1 double

—— The PCIe2 x16 link allows 1 server to access 2 GPUs

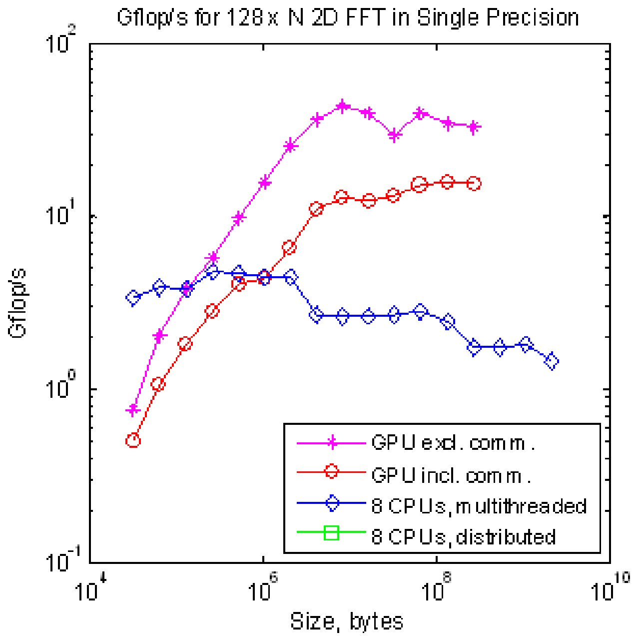
GPGPU in MATLAB: Easy and Fast… but Limited

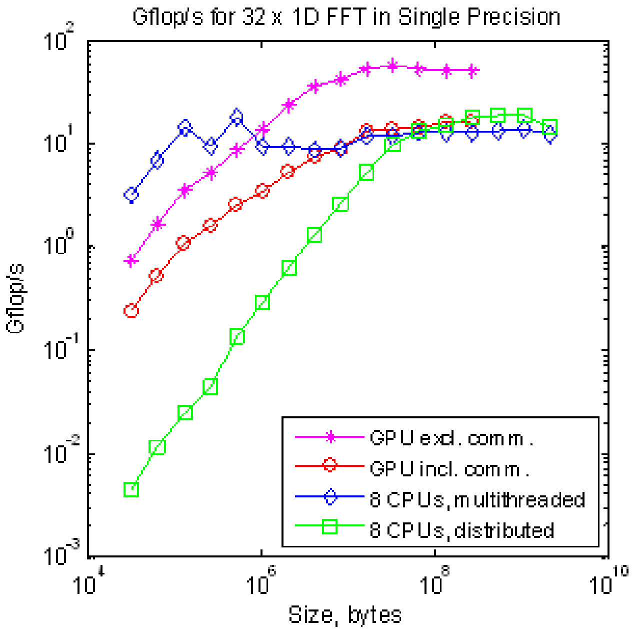
- New feature in MATLAB R2010b: **gpuArray** datatype, operations
- To use the GPU, MATLAB code changes are trivial
  - Move data to GPU by declaring a gpuArray
  - Methods like fft() are overloaded to use internal CUDA code on gpuArrays

```
g = gpuArray(r);
f = fft2(g);
```

- Initial benchmarking with large 1D and 2D FFTs shows excellent acceleration on 1 GPU vs. 8 CPU cores
  - Including communication: up to 10x speedup
  - Excluding communication: up to 20x speedup
- BUT only a few intensive matrix operations like fft() are overloaded

GPU Definitely Excels at Large FFTs in MATLAB





- 2D FFT > 8 MB can be 9x faster on GPU (including data transfers), but array of 1D FFTs is equally fast on 8 cores
- Limited to 256 MB due to bug in cuFFT 3.1; fixed in 3.2