# Data Analysis with MATLAB

Steve Lantz
Senior Research Associate
Cornell CAC

*Workshop: Data Analysis on Ranger, January 19, 2012*

# MATLAB Has Many Capabilities for Data Analysis

- Preprocessing (*sift it!*)
  - Scaling and averaging
  - Interpolating and decimating
  - Clipping and thresholding
  - Extracting sections of data
  - Smoothing and filtering
- Applying numerical and mathematical operations (*crunch it!*)
  - 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

*MATLAB can be useful when your analysis needs go well beyond visualization*

# 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
  - Images in many different formats
  - 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
  - dlmread/dlmwrite
  - xmlread/xmlwrite
  - csvread
  - xlsread
  - imread
- See “help iofun” for more

- Low Level Routines…
- 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

# Support for Scientific Data Formats

- HDF5 (plus read-only capabilities for HDF4)
  - h5disp, h5info, h5read, h5readatt
  - h5create, h5write, 5writeatt
- NetCDF (plus similar capabilities for CDF)
  - ncdisp, ncinfo, ncread, ncreadatt
  - nccreate, ncwrite, ncwriteatt
  - netcdf.funcname provides lots of other functionality
- FITS – astronomical data
  - fitsinfo, fitsread
- Band-Interleaved Data

# 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')
```

# Options for Sharing Results

- Push the "publish" button to create html, doc, etc. from a .m file
  - Feature has been around 6 years or so
  - Plots become embedded as graphics
  - Section headings are taken from cell headings
    - 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 the 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

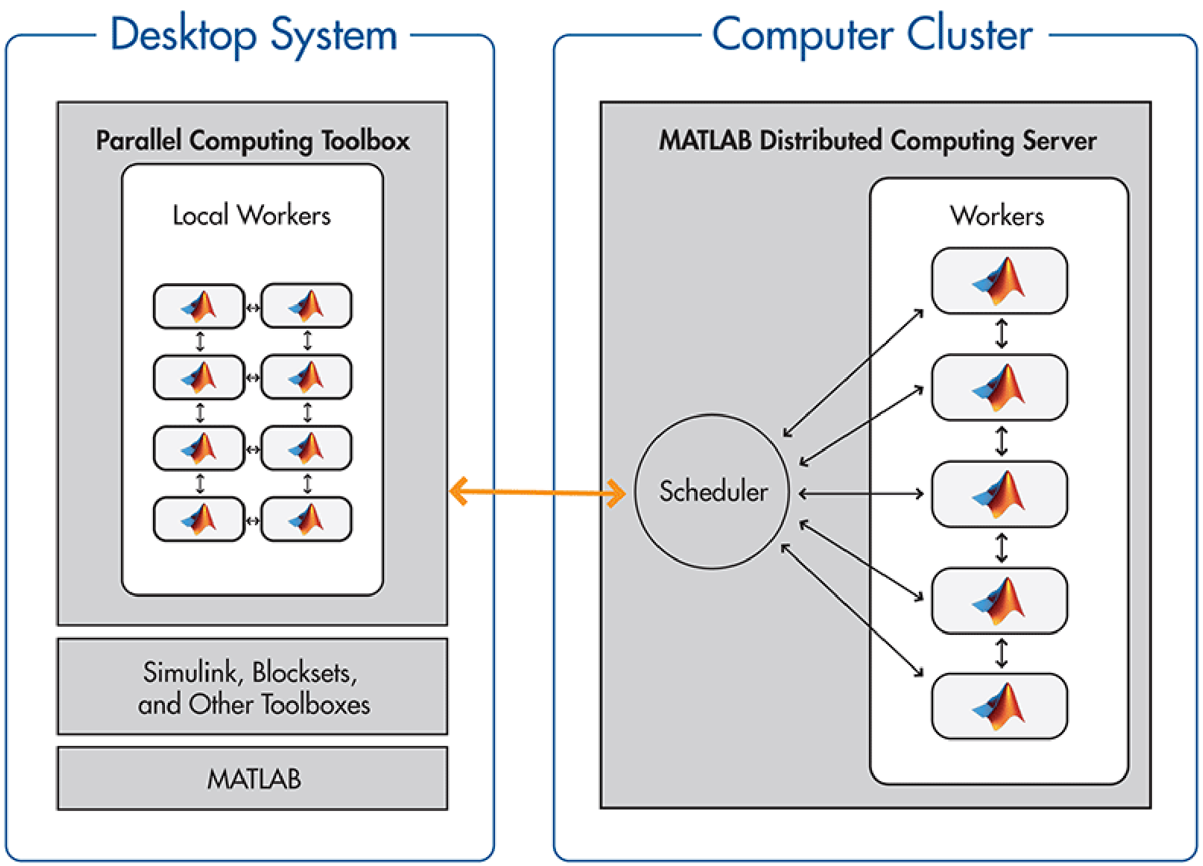
```
function nicedays = count_nicedays( yr )
%COUNT_NICEDAYS returns number of days with a high between 70 and 79.
%   It assumes data for the given year are found in a specific file
%   that has been scraped from the Ithaca Climate Page at the NRCC.

% 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)
  - Multiple distributed runs of a sequential function (createJob)
  - Single program, multiple data (spmd, createParallelJob)
  - Parallel code constructs and algorithms in the style of MPI
  - Codistributed arrays, for big-data parallelism
- 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 local 2
parfor i=1:3
count_nicedays(2005+i)
end
```

- Note, matlabpool starts extra MATLAB workers or “labs” – the size of the worker pool is set by the default “local” configuration – usually it’s the number of cores (e.g., 2 or 4), but the license allows 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)

# A Different Way to Do the Same Thing: createJob

- Try the following code, which runs 3 distributed (independent) tasks on the local “labs”.  The 3 tasks run concurrently, each taking one of the supplied input arguments.

```
matlabpool close
sched = findResource('scheduler','configuration','local');
job = createJob(sched)
createTask(job,@count_nicedays,1,{{2006},{2007},{2008}})
submit(job)
wait(job)
getAllOutputArguments(job)
```

- If only 2 cores are present on your local machine, the 3 tasks will share the available resources until they finish

# How to Do Nearly the Same Thing Without PCT

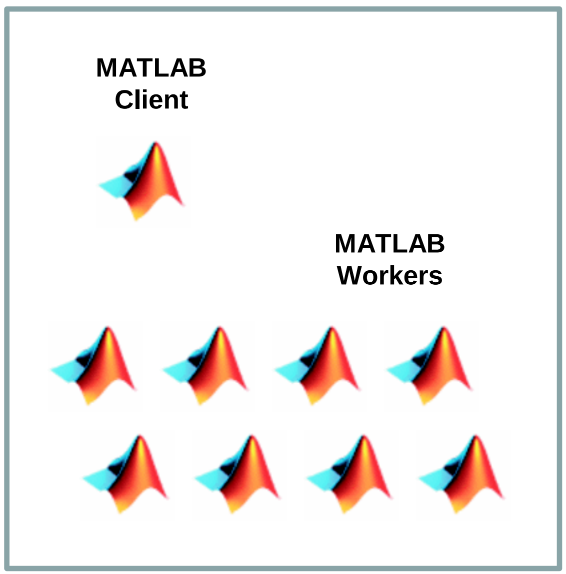
- Create a MATLAB .m file that takes one or more input parameters
  - The parameter may be the name of an input file, e.g.
- Use the MATLAB C/C++ compiler (mcc) to convert the script to a standalone executable
- Run N copies of the executable on an N-core machine, each with a different input parameter
  - 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

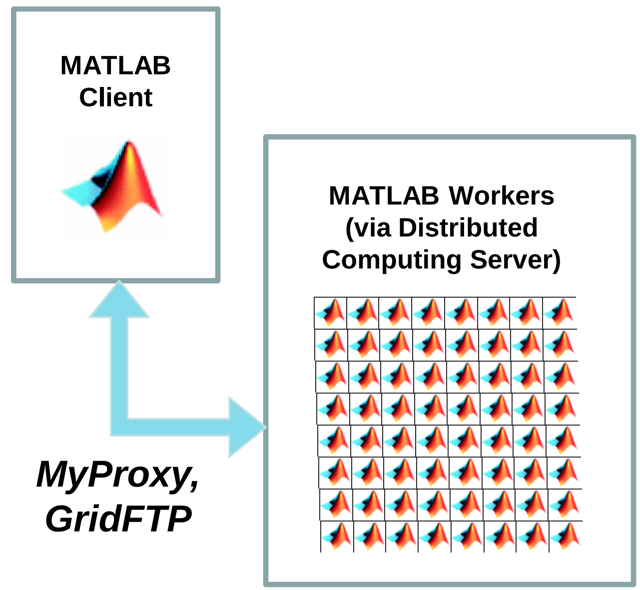
- Over 150 MATLAB functions are overloaded for codistributed arrays
  - Such arrays are actually split among mutliple MATLAB workers
  - In the command window, just type the usual e = d*c;
  - Under the covers, the matrix multiply is executed in parallel using MPI
  - Some variables are cluster variables, 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
  - createParallelJob(sched), submit(job) for parallel tasks
  - Many MPI functions have been given MATLAB bindings, e.g., labSendReceive, labBroadcast; these work on all datatypes

# Red Cloud with MATLAB: New Way to Use the PCT

CAC's client software extends the Parallel Computing Toolbox!




*Select the local scheduler – code runs on client CPUs*



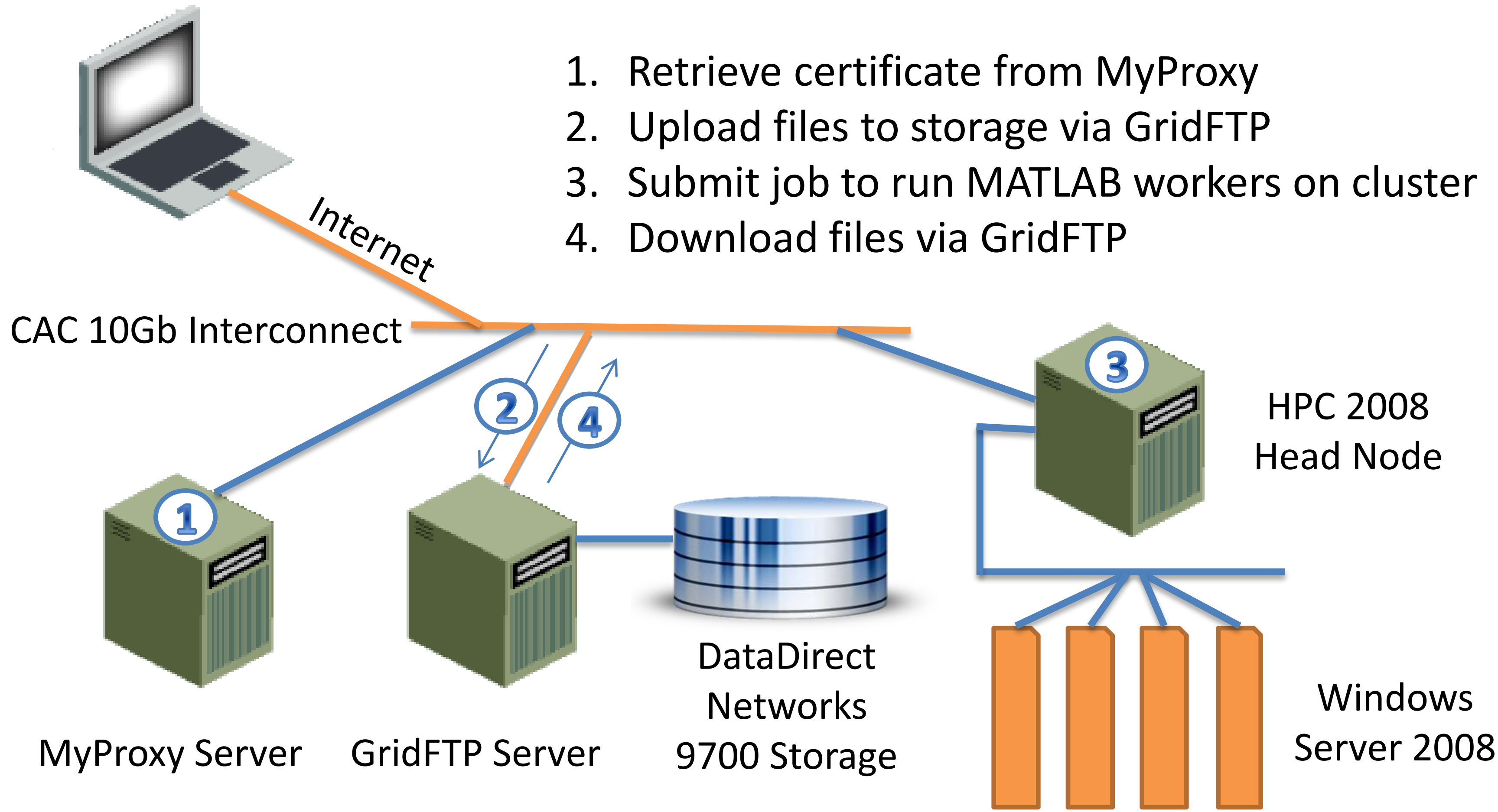

*Select the CAC scheduler – Code runs on remote CPUs*

# Red Cloud with MATLAB: 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

# Red Cloud with MATLAB: Hardware View

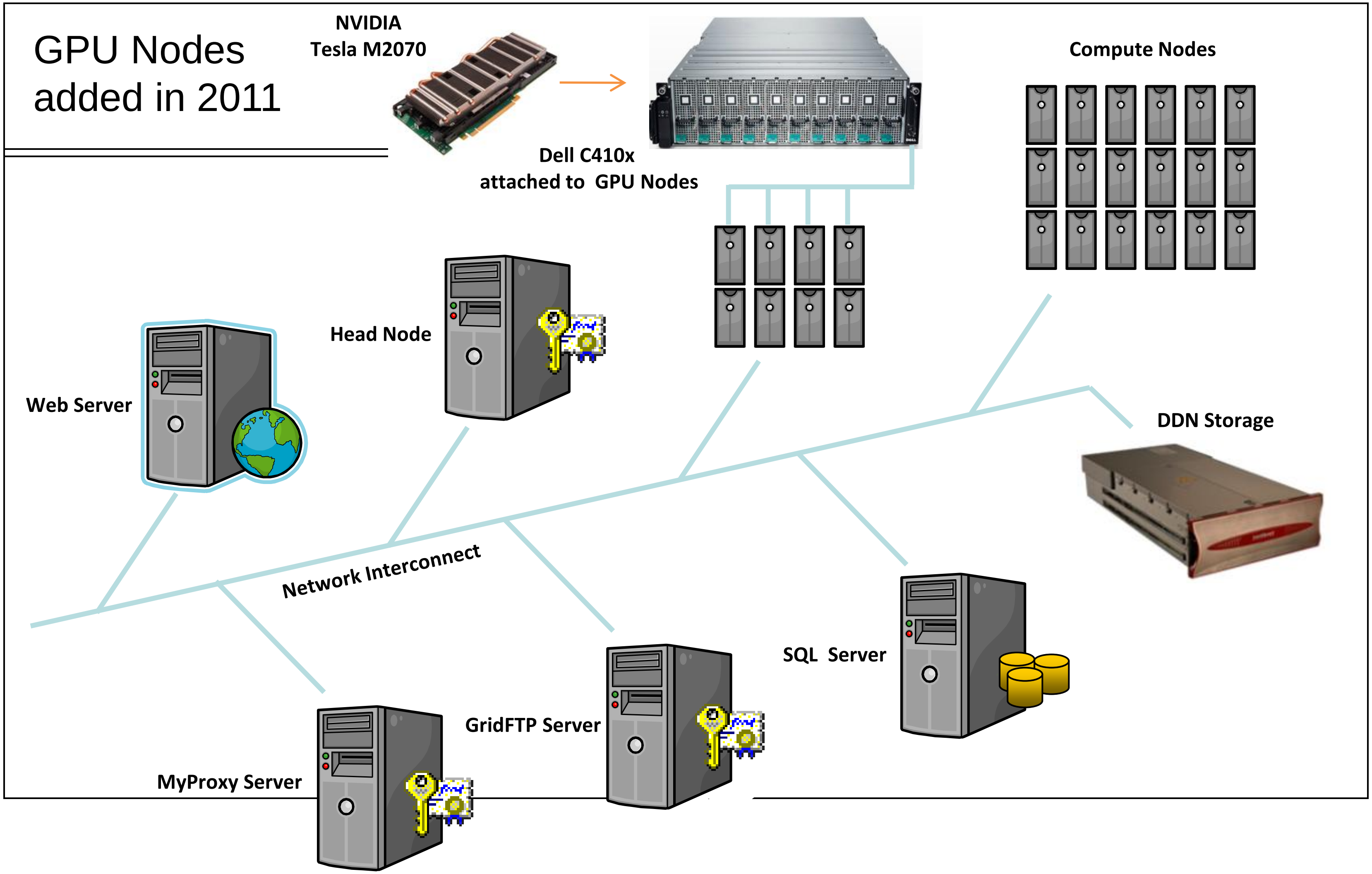
1. Retrieve certificate from MyProxy
2. Upload files to storage via GridFTP
3. Submit job to run MATLAB workers on cluster
4. Download files via GridFTP



# Red Cloud with MATLAB: System Specifications

- Initial configuration: 64 Intel cores in Dell C6100 rack servers
  - Total of sixteen 2.4 GHz Xeon E5620 processors (4 cores each)
  - 52 cores in Default queue, 4 in Quick queue, 8 in GPU queue
  - 2 GB/core in Default and Quick queues; 10 GB/core in GPU queue
- Special feature: 8 NVIDIA Tesla M2070 GPUs (in Dell C410x)
  - Each Tesla runs at up to 1 Tflop/s and has 6 GB RAM
- Cluster OS: Microsoft Windows HPC Server 2008 R2
  - Supports MATLAB clients on Windows, Mac, and Linux
- Includes 50 GB DataDirect Networks storage (can be augmented)
  - RAID-6 with on-the-fly read/write error correction
  - Accessible to cores at 1 Gb/s; up to 10 Gb/s externally via GridFTP
- Request an account at http://www.cac.cornell.edu/RedCloud

# System Architecture

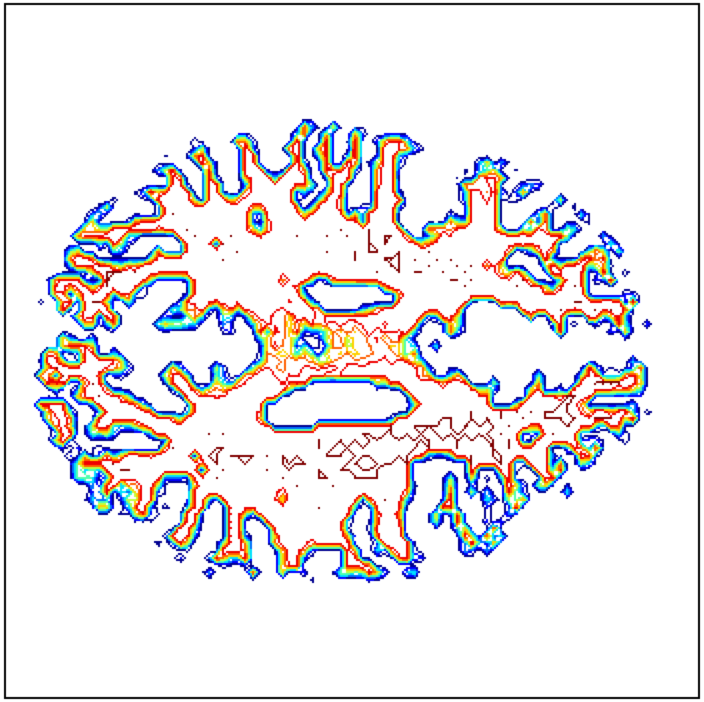


# Case Study: Analysis of MRI Brain Scans

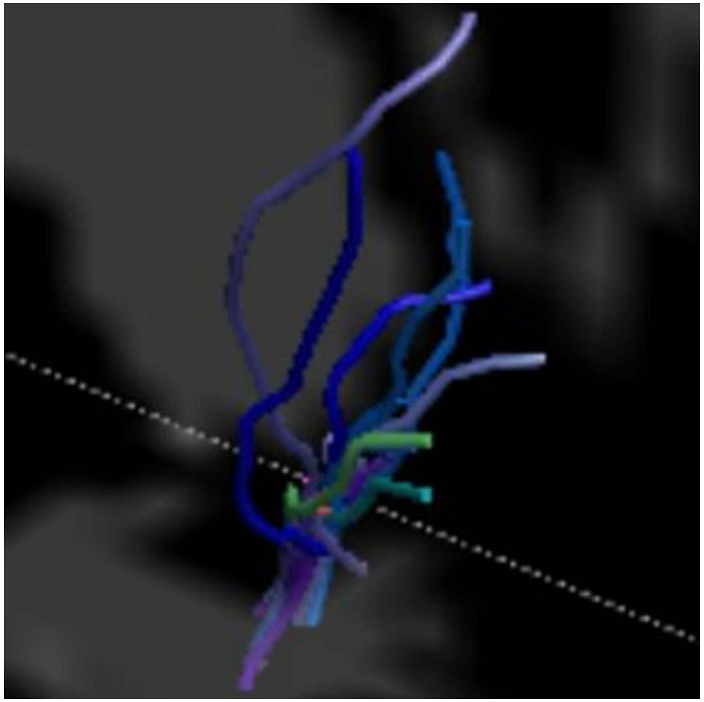
- Work by Ashish Raj and Miloš Ivković, Weill-Cornell Medical College
- Research question: Given two different regions of the human brain, how interconnected are they?
- Potential impact of this technology:
  - Study of normal brain function
  - Understanding medical conditions that damage brain connections, 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

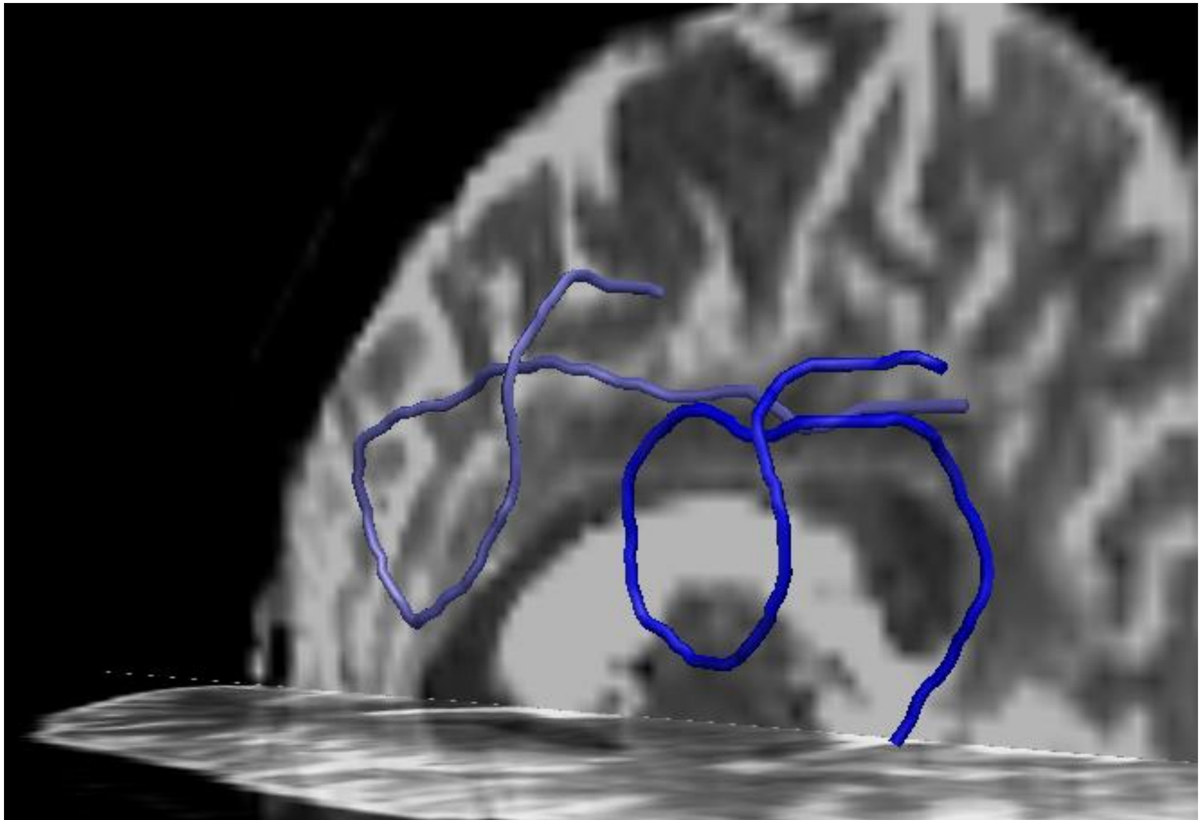


- Fiber tracts to show lines of preferential diffusion



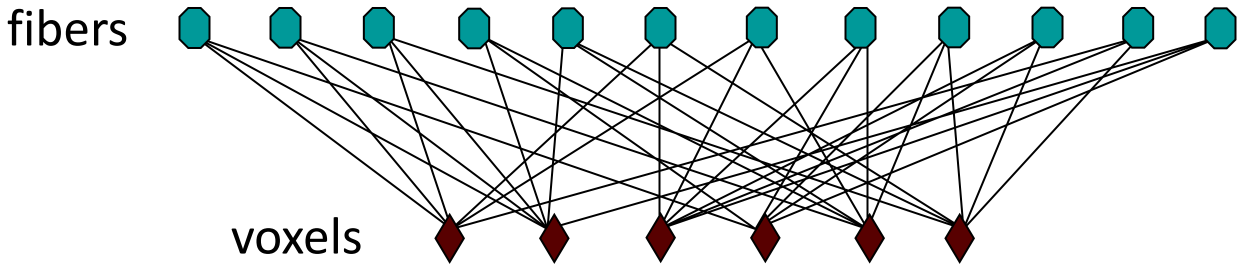
# Need for Computational Power

- 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 and voxels, edge weights = connection strength

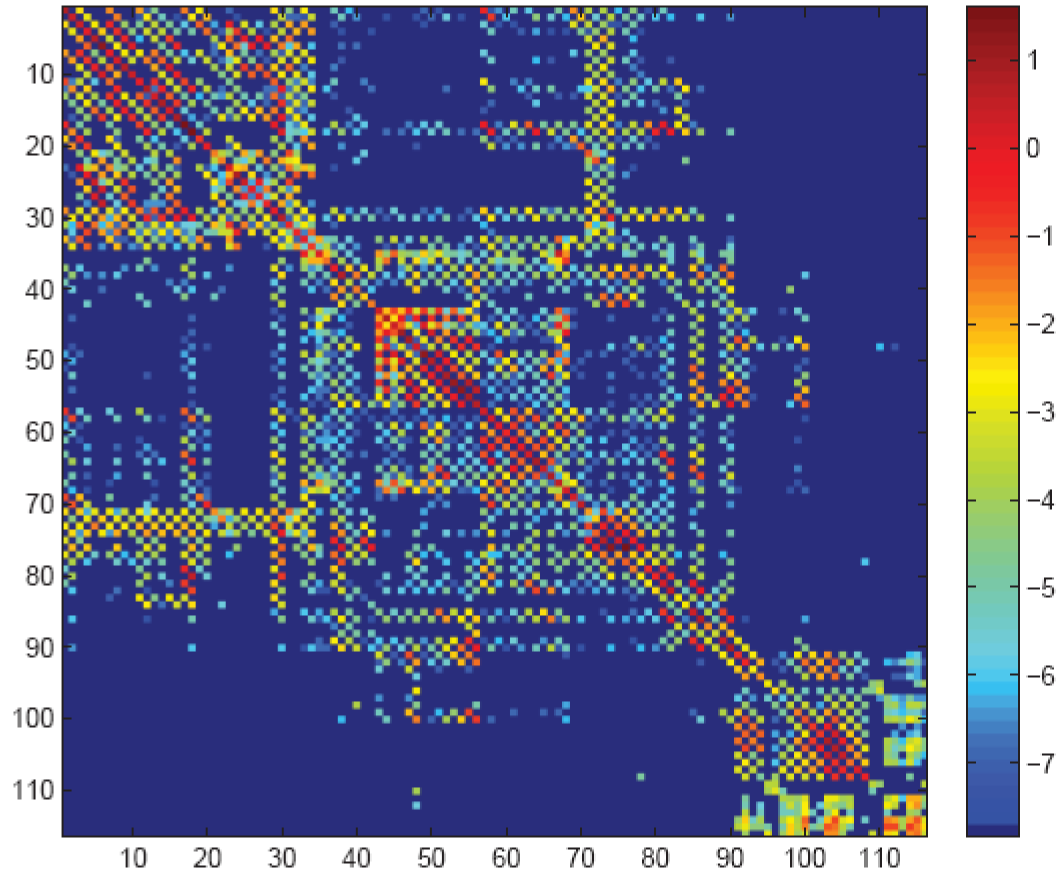



- MATLAB computations at each voxel are independent of all other voxels, likewise for fibers; *inherently parallel*

# Data Product: Connectivity Matrix

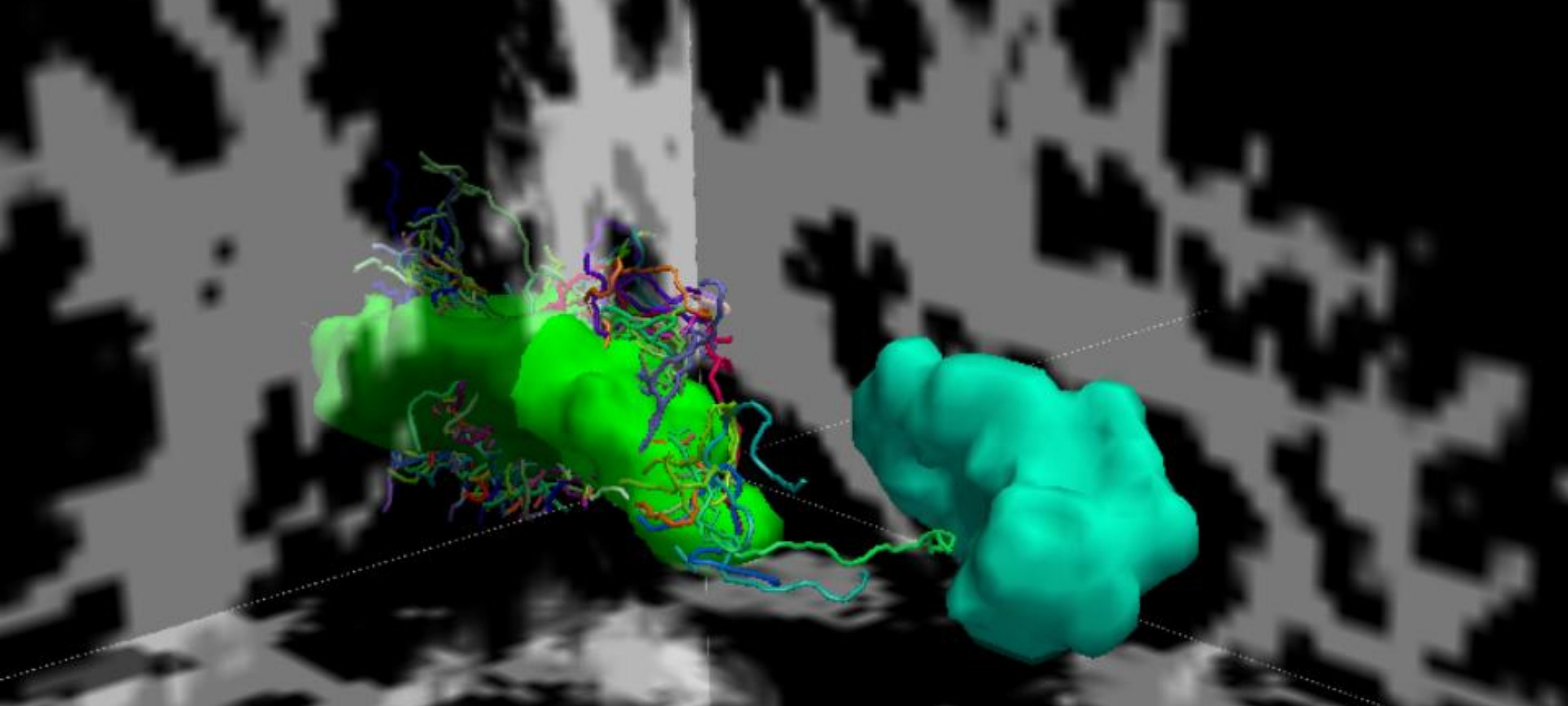
- Graph with 360K nodes, 1.8M edges, optimized in 1K iterations

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



Cornell University
Center for Advanced Computing

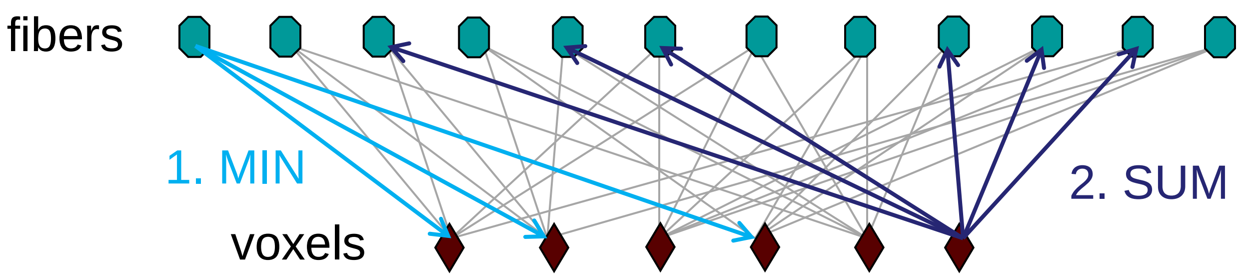
# Result: Better 3D Structure



*Analysis finds the most important connections between brain regions*

# Message-Passing Algorithm

- Iterative procedure also known as “min-sum”
- Fiber-centric step: for each fiber, find the minimum of all its edge weights; reset the edges to that value (or to the second smallest value, if already at min)



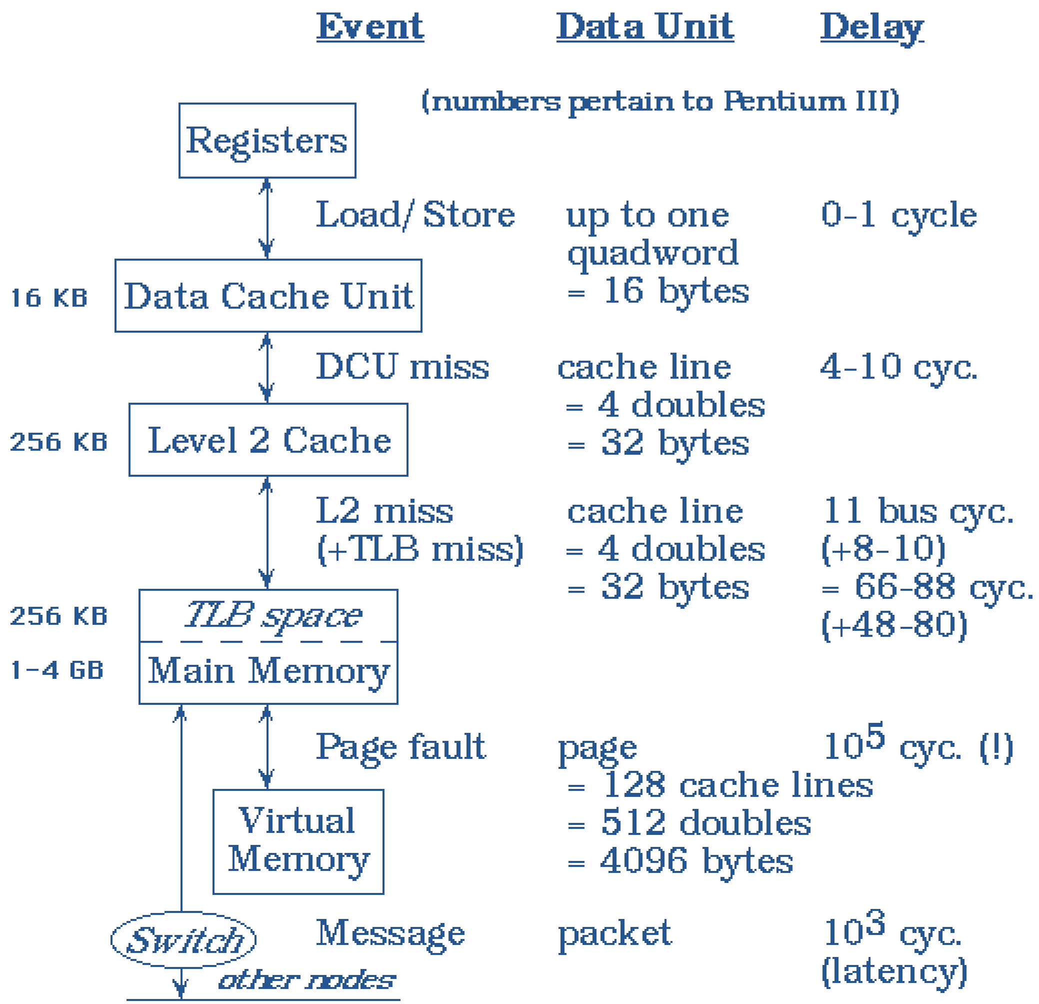

- Voxel-centric step: for each voxel, sum up its current edge weights; distribute WM value back proportionately

# Round One: Parallelization

- Min can be computed independently for each fiber
- Sum can be computed independently for each voxel
- Loops over fibers and voxels can be converted into “parfor” or parallel-for loops in MATLAB PCT (R2011b)
  - On 8 cores: 375 sec/iteration goes down to 136 sec/iteration
  - After pre-packing the WM data structure to include only voxels traversed by at least one fiber: 42 sec/iteration
  - By eliminating repeated searches through improved indexing: 32 sec/iteration, *without parfor*
- Good memory locality and a better algorithm beat parallelization!

# The Lessons of Memory Hierarchy

- Stay near the top of the hierarchy: the further down you go, the costlier a fetch becomes
- Keep data in cache as long as possible
- Take small strides, preferably stride-1 (contiguous), to make full use of cache lines



# MATLAB Loves Matrices

- Original code was written using **structs**
  - Advantage: little wasted space; handles variable-length lists of edges connected to a voxel (1–274) or fiber (2–50)
  - Disadvantage: poor data locality, because structs hold lots of extraneous info about voxels/fibers
  - Disadvantage: unsupported on GPU in MATLAB
- Better to store data in **matrices**
  - Column-wise operations on a matrix are often multithreaded in the MATLAB core library; no programmer effort required
  - Implication: easily get "vectorized" performance on CPUs or GPUs by converting loops into matrix operations

# Round Two: Vectorization

- So, just throw everything into one giant matrix?
  - First problem: row-major ordering = bad stride
  - Second problem: mixing of dissimilar data = poor data locality
  - Due to these problems, the initial matrix-based version of the serial min-sum algorithm ran slower, 53 sec/iteration
  - Yet another lesson of memory hierarchy (for a collaborator)
- First optimization steps were easy…
  - Make *columns* receive all edge weights (messages) pertaining to one voxel or fiber—MATLAB stores in column-major order
  - Pull out only necessary info and store in separate, condensed matrices

# Round Three: CPU Optimization

- Tighten up memory utilization by grouping fibers and voxels according to numbers of coordinating edges
  - Different matrices for fibers that connect to 2, 3, 4… edges
  - Now have full columns in the matrix for all 2-edge fibers, etc.
  - Put the series of matrices into a “cell array” for easy reference
- Resulting code is much more complex
  - New inner for-loops over fiber count, voxel count
  - Challenge to build the necessary indexing
- Excellent performance in the end: **0.25 sec/iteration**
- Good outcome, but days and days of work by Eric Chen

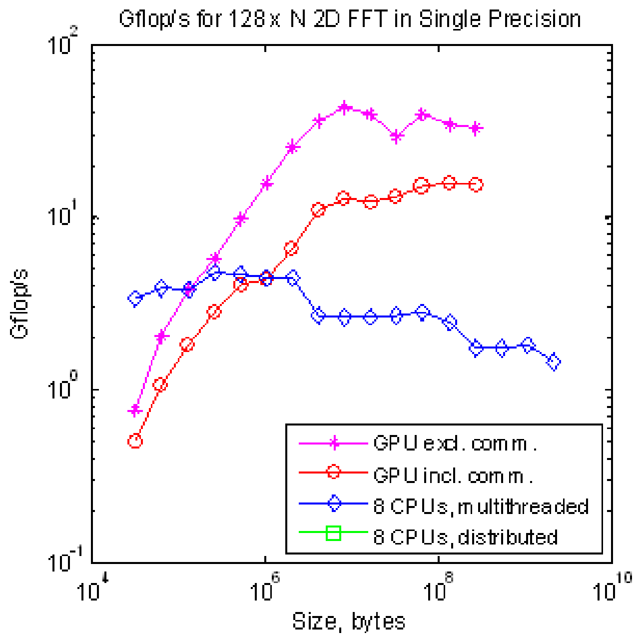
# New Idea: GPGPU in MATLAB

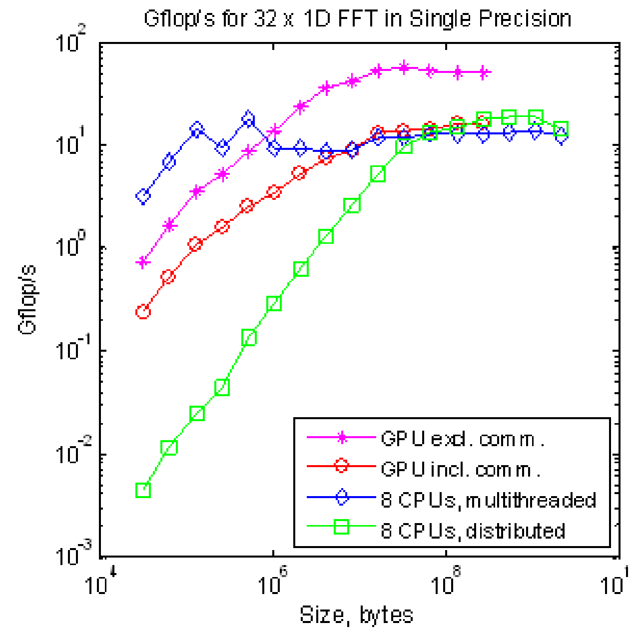
- New feature in MATLAB R2010b: **gpuArray** datatype, operations
- To use the GPU, MATLAB code changes are trivial
  - Move data to GPU by declaring a gpuArray
  - Methods like fft() are overloaded to use internal CUDA code on gpuArrays

```
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
- Easy and fast… BUT can it help with the particular data analysis?

# 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

# Round Four: GPU Optimization

- In R2011b, min and sum can use MATLAB’s built-in CUDA code!
- Go back to big, simple matrices with top-heavy columns
  - Reason 1: GPU doesn’t deal well with nested for-loops
  - Reason 2: Want vectorized or SIMD operations on millions of items
- Resulting code is actually *less* complex
  - Keep data in a few huge arrays
  - Move them to the GPU with gpuArray()
  - Functions min and sum are overloaded (polymorphic), so no further code changes are needed
- Best result (after a few tricks): **0.15 sec/iteration**
  - 350x speedup over initial matrix-based version
  - 2500x speedup over initial struct-based version

# Is It Really That Simple?

- No. The GPU portion of MATLAB PCT is evolving rapidly.
  - A year ago, the move to GPU was impossible: subscripting into arrays wasn't allowed, min was completely absent, etc.
  - Now these operations are present and work well, but gaps still remain; e.g., min does not return the location of the minima as it does on the CPU, and a workaround was needed for the GPU.
- Your application must meet two important criteria.
  - All required operations must be implemented natively for type GPUArray, so your data seldom have to leave the GPU.
  - The overall working dataset must be large enough to exploit 100s of thread processors without exceeding GPU memory.

# Implications for Data Analysis in MATLAB

- The MATLAB Parallel Computing Toolbox has a variety of features that can dramatically speed up the analysis of large datasets
- New GPU functionality is a good addition to the arsenal
- A learning curve must be climbed…
  - General knowledge of parallel and vector computing can be helpful for restructuring the compute-intensive portions of a code
  - Specific knowledge of PCT functions is needed to exploit features
- But speed matters!…
  - MRI image analysis has mostly been of interest to medical researchers
  - Now it can potentially move into the realm of a diagnostic tool for real-time, clinical use
  - Modest hardware requirements may make such computations feasible