A Hybrid CPU-GPU System for Stitching Large Scale Optical Microscopy Images

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- Video games & special effects industries

Contents

Computing as an Enabler of Measurements

Goals & Objectives

Goals

- Computing as enabler & accelerator of metrology
  - Biology, Materials Science…
  - Third leg of Science
- Computationally steerable experiments

Themes

- Computational measurements
  - Augment physical measurements
- Performance
  - Computing-based measurements in "real-time"

Change Drivers

- Dramatic increases in computing power
  - Desktop supercomputer!
- Dramatic increases in storage
- Automated data collection

What $8K gets you (Sep 2011)?

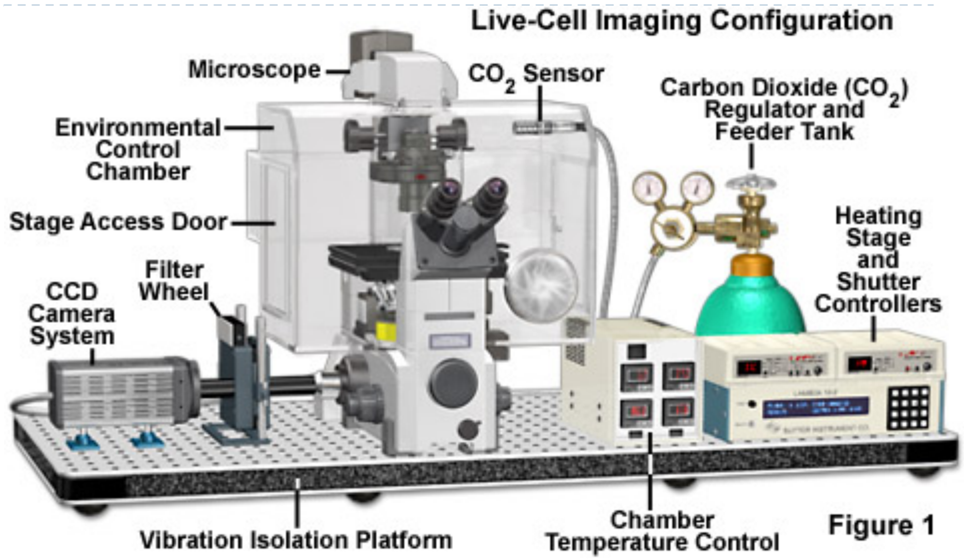
- 2 Intel quad-core Xeon E5620 2.4 GHz
  - 2 threads per core
  - Peak 38.4 GFLOPS
- 24 GB RAM
- 2 Nvidia Tesla C2070
  - 448 cores & 6 GB each
  - Peak 2 x 515 GFLOPS
- 1 Nvidia Quadro 4000
  - 256 cores
  - Peak 486.4 GFLOPS
- ~ 1.5 TFLOPS!

- June 2005 Top500:
  - R_{peak}: 1.28–183.5 TFLOPS
  - NEC SX-5/128M8 3.2ns

Desktop Supercomputer

Life Sciences

- High end microscopes:
  - Reaches $150–200K!
  - Nikon Live Cell Imaging station (URL)



- Prediction:
  - Will come with a desktop supercomputer.

Transformative Moment

- Current request:
  - Make my work easier.
- Strategic goal:
  - Change the way scientists work & discover!
- Approach:
  - Massive data & compute driven techniques.
    - Processing & data collection rates *= 100–1000.

Accelerators in HPC

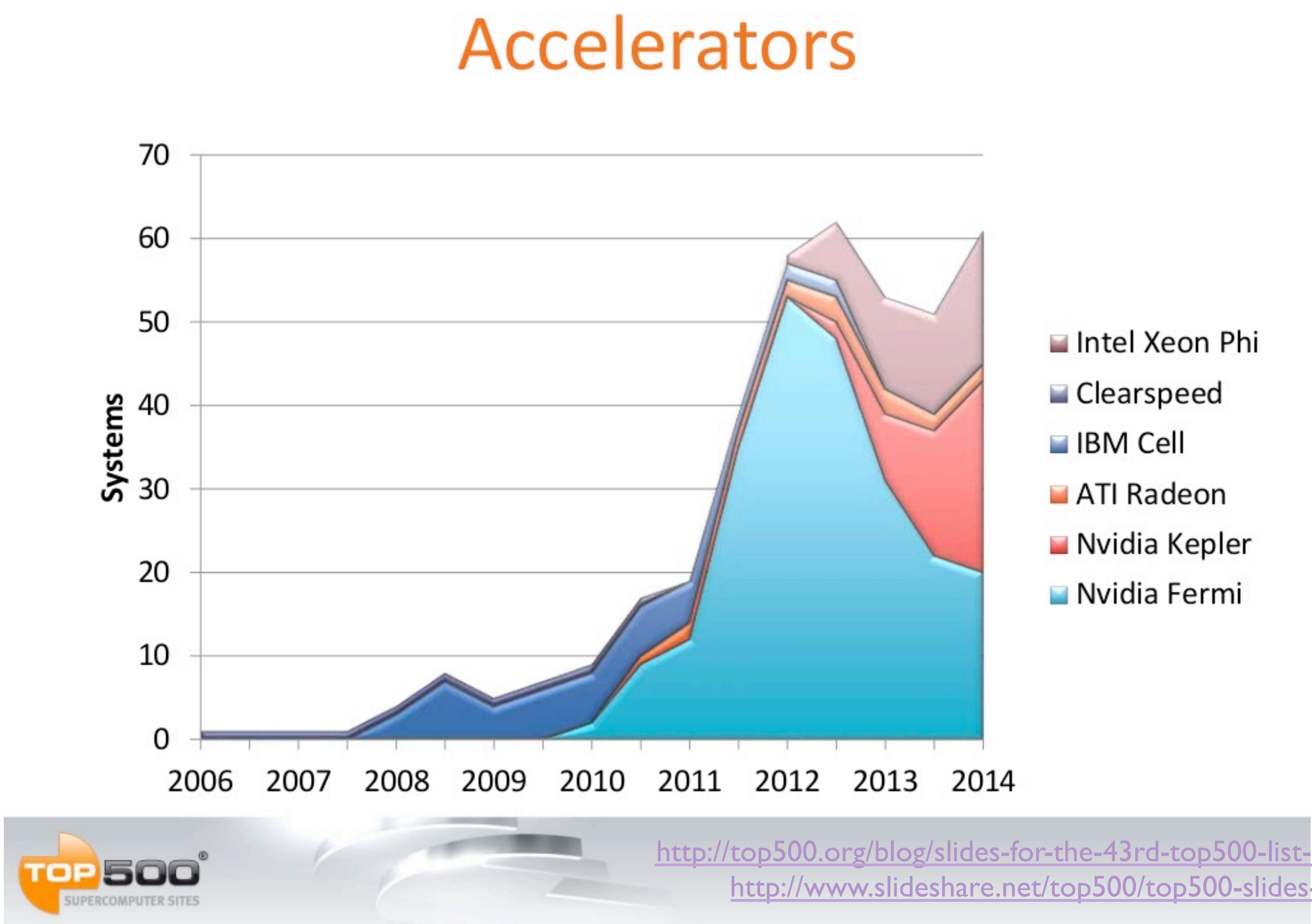
Top500 List (June 2014)

- Released twice a year (ISC & SC)

- 4 of Top 10 machines use accelerators
  - Intel Phi: Tianhe-2 (#1), Stampede (#7)
  - NVIDIA GPUs: Titan (#2), Piz Daint (#6)

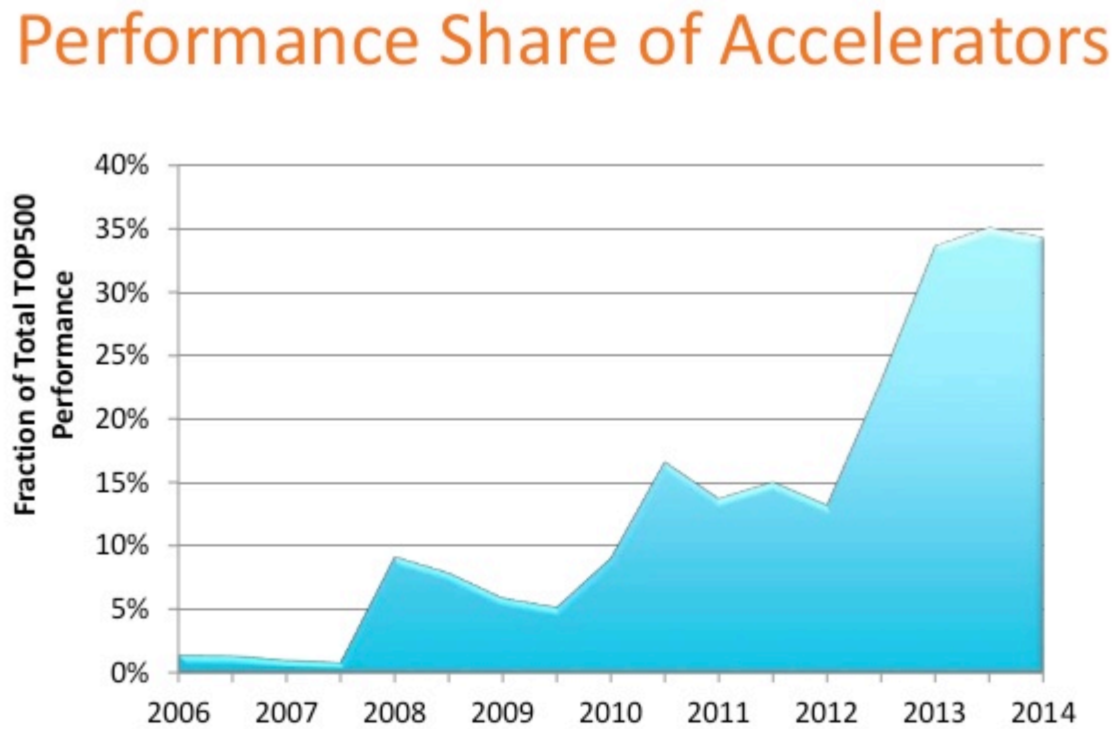
- 62 of Top 500 machines:
  - Nov 2013 edition had 53
  - NVIDIA GPUs: 44; ATI GPUs: 2
  - Intel Phi: 17

Top500 Accelerators (June 2014)



http://top500.org/blog/slides-for-the-43rd-top500-list-now-available/
http://www.slideshare.net/top500/top500-slides-for-june-2014

Top500 Accelerators (June 2014)



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http://www.slideshare.net/top500/top500-slides-for-june-2014

Recent Announcements (SC'14)

- DOE's Summit (ORNL) and Sierra (LLNL)
- IBM Power9 CPUs
- NVIDIA Volta-based Tesla GPUs
  - Architectures: Kepler, Maxwell, Pascal, Volta
- Mellanox EDR Infiniband
- Summit: 3400 nodes, 150--300 PFLOPS (~ 10MW)
  - Would appear on Top500 list with 4 nodes only!

NVIDIA Tesla K80

- Dual Tesla K40 card, $5K
  - NVIDIA Kepler GK210 architecture
- 2 x 2496 CUDA Cores
- Clock up to 562--875 MHz
- Memory:
  - 2 x 12 GB GDDR5
  - 2 x 384 GB/s internal bandwidth
- 300W Minimum System Power
  - Passive cooling
- Single precision: 5.6--8.75 TFLOPS
  - Double precision: 1.87--2.91 TFLOPS

Announced at SC'14

More Changes Coming

- AMD's APU
  - Combines CPU & GPU cores
- ARM's big.LITTLE
- Intel's Knights Landing
  - CPU + Xeon Phi cores on same die
  - Share memory bandwidth
- NVIDIA Pascal
  - NVLink, 3D stacked memory

Image Stitching for Optical Microscopy

Image Stitching for Optical Microscopy

Objectives

- Stitching of optical microscopy images at *interactive* rates
- General purpose library, ImageJ/Fiji plug-in, etc.
- Stitch & visualize plate between repeat experiments
  - Up to ~50 min to image a plate
  - Image plate every 1 hour

Success criterion

- Transformative impact
  - Run sample problem in < 1 min
  - > 10–100x speed improvement

Image Stitching Problem

- Optical microscopes scan a plate and take overlapping partial images (tiles)
- Need to assemble image tiles into one large image
  - Software tools
- Modern microscopy automated:
  - Scientists are acquiring & processing large sets of images

Starting Point

- ImageJ/Fiji
  - Open source Java
  - Multithreaded
- NIST prototype
  - MATLAB
- NIST data set:
  - 59x42 images (~ 7 GB)
- Hardware:
  - 2 Xeon quad-core CPUs
  - 48 GB
  - 2 NVIDIA Tesla 2070 GPUs

	ImageJ Fiji	NIST prototype
Old H/W		50 min
New H/W	~ 3.6 h	17 min

Motivation

- Proof of concept application
  - Illustrate benefits of desktop supercomputing
    - Multicore and GPU computing
- Heavy computing workloads

  > high-end desktop or small server

  < cluster

Data Set

- Grid of 59x42 images (2478)
- 1392x1040 16-bit grayscale images (2.8 MB per image)
  - ~ 7 GB

- Source:
  - Kiran Bhadriraju (NIST, Univ. of Maryland)

Evaluation Platform

Hardware

- Dual Intel® Xeon® E-5620 CPUs (quad-core, 2.4 GHz, hyper-threading)
- 48 GB RAM
- Dual NVIDIA® Tesla™ C2070 cards

Reference Implementations

- ImageJ/Fiji™ Stitching plugin, ~ 3.7 h
- MATLAB® prototype, ~17.5 min on a similar machine

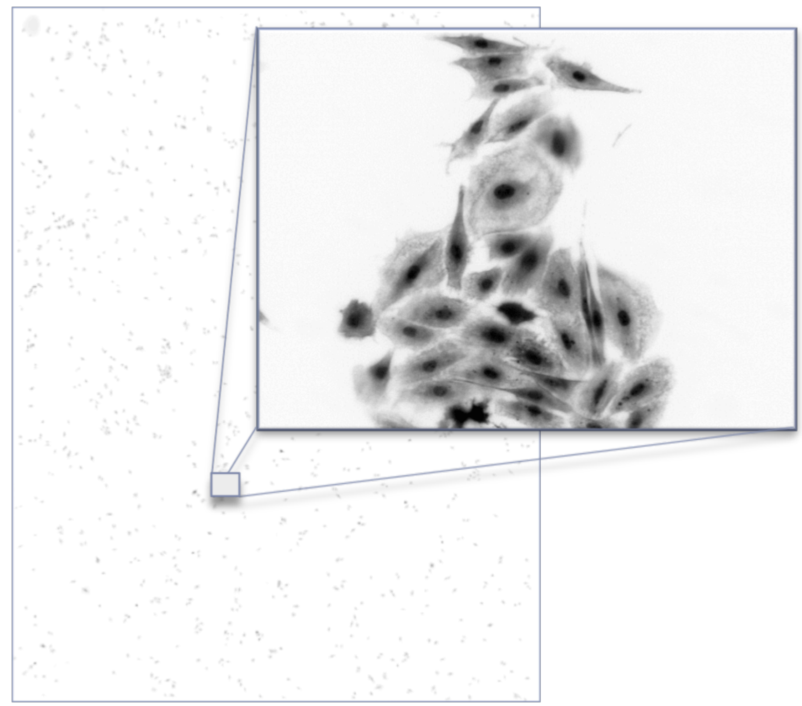
Software

- Ubuntu Linux 12.04/x86_64, kernel 3.2.0
- Libc6 2.1.5, libstd++6 4.6
- BOOST 1.48, FFTW 3.3, libTIFF4
- NVIDIA CUDA & CUFFT 5.0

Image Stitching Problem…

Three phases:

1. Compute the X & Y translations for all tiles
   - Produces over-constrained system
2. Remove over-constraint
   - Use global optimization techniques
3. Apply the translations & compose the stitched image

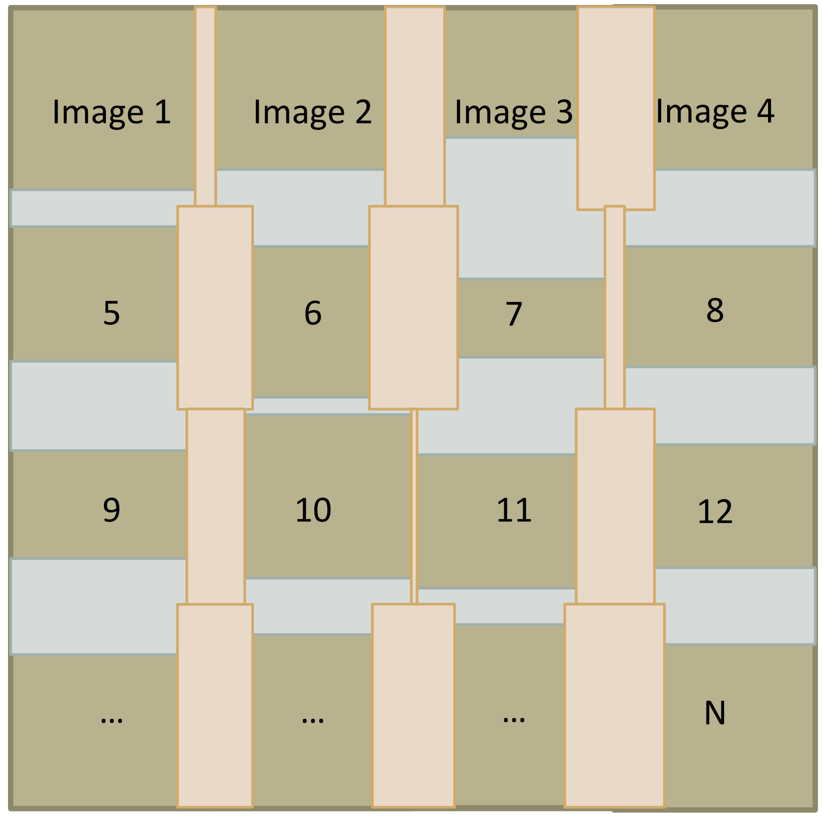


- Main focus is on phase 1

Image Stitching Algorithm

Loop over all images:

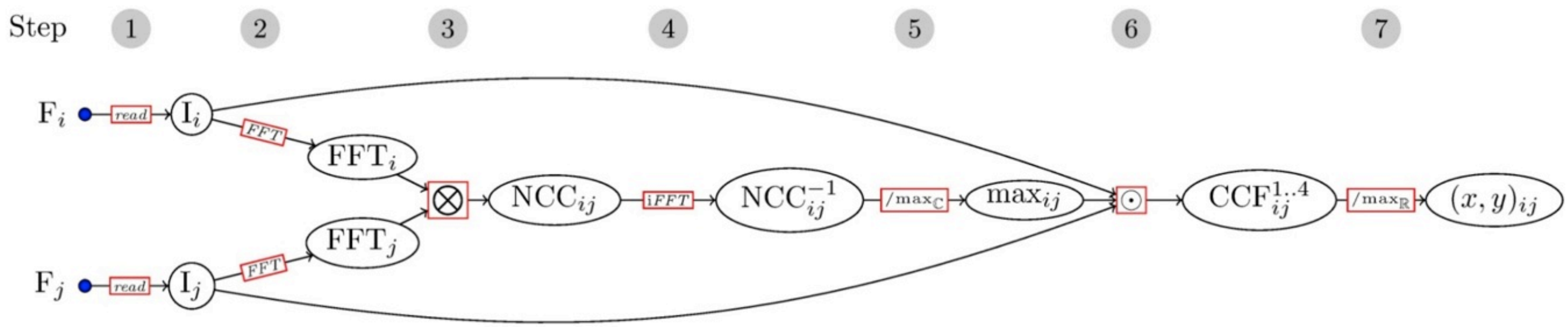
- Read an image tile
- Compute its FFT-2D
- Compute correlation coefficients with west and north neighbors
  - Depends on FFT-2D for each tile

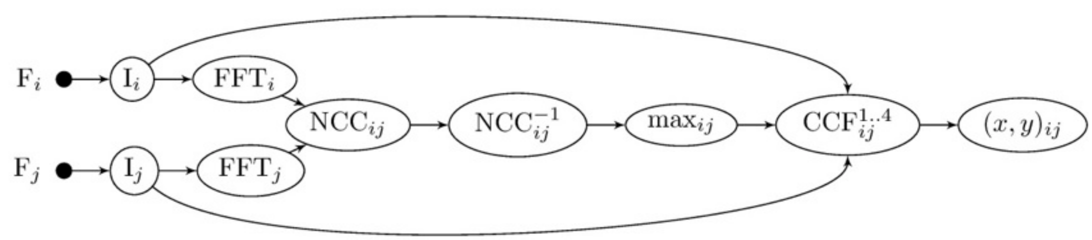


Major compute portions:

- FFT-2D of tiles
- Compute and normalize phase correlation
- Inverse FFT-2D
- Max reduction of correlation

Image Stitching Algorithm…





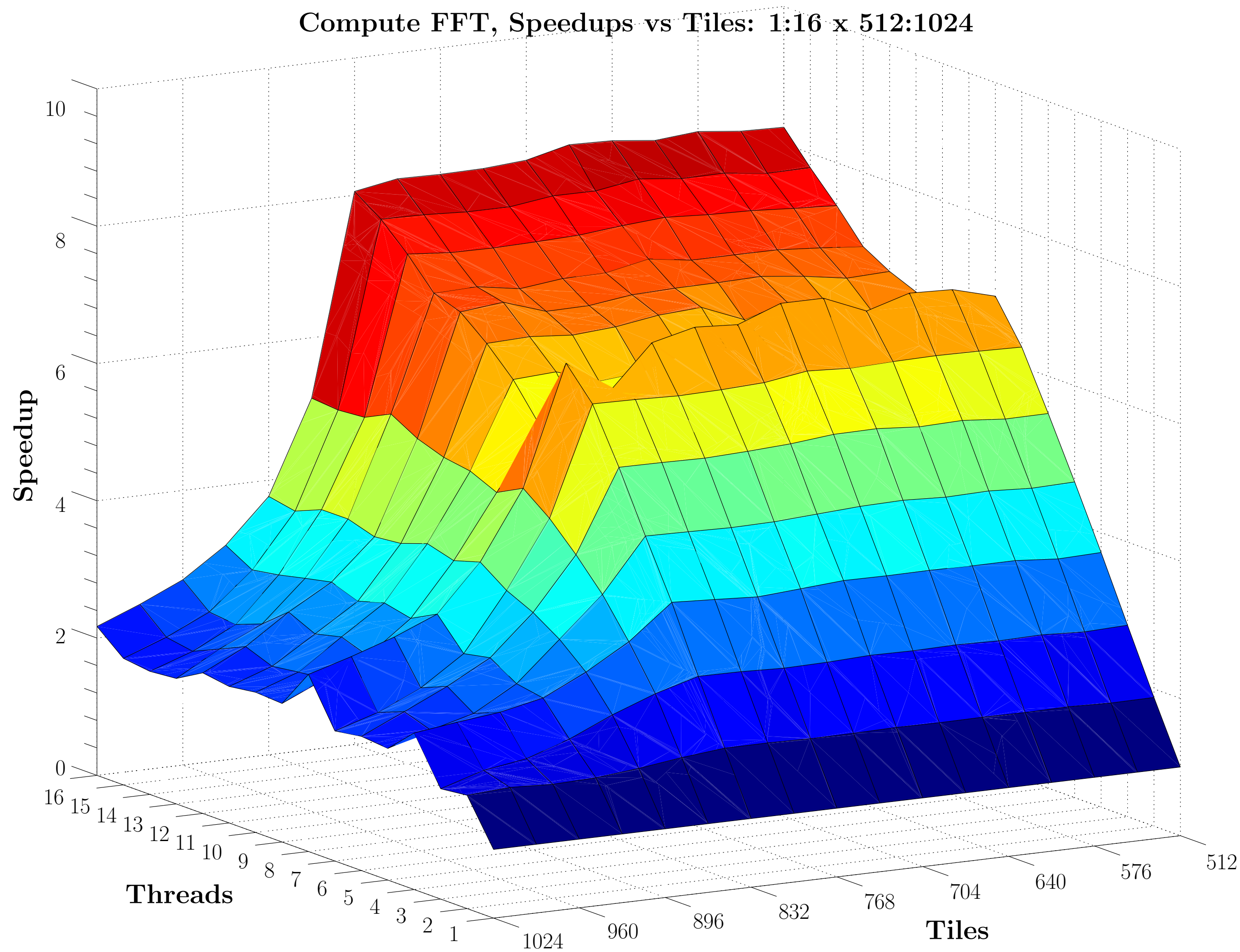
Algorithm's Parallel Characteristics

- Almost embarrassingly parallel
  - Large number of independent computations
  - For an *n* x *m* grid:
    - FFT for all images nxm
    - NCC for all image pairs $2nxm - n - m$
    - FFT^{-1} for the NCCs of all image pairs $2nxm - n - m$
    - …
- Caveats
  - Data dependencies
  - Limited memory

Memory Limitations

- Image tile:
  - 1040 x 1392 2-byte pixels: 2.76 MB
- Image transform
  - 1040 x 1392 x 16 = 22.1 MB
- Forward transforms for all tiles:
  - 22.1 MB x 59 x 42 = 53.5 GB!

Memory Limitations…



Performance-Driven Development Approach

- Extends *Edit-Compile-Debug* Cycle:
  - Edit-compile-debug
  - Measure performance
    - Identify bottleneck
  - Modify design

- Performance measurements
  - Execution time on a lightly loaded machine
    - Repeat timings, drop high & low values
  - Metered data structures
    - Examples: maximum & average queue lengths

Development Approach…

- Three main branches
  - Share code + utilities, regression tests…
  - Sequential
  - Pure multicore
  - Hybrid CPU-GPU
- Java plugin
  - Targeted for release in Feb 2015.

Implementations & Results

		Time	Speedup	*Effective* Speedup	Threads
CPU only	Sequential	10.6 min		20.3x	1
	Simple Multi-Threaded	1.6 min	6.6x	135x	16
	Pipelined Multi-Threaded	1.4 min	7.5x	154x	16
CPU-GPU	Simple GPU	9.3 min	1.14x	23.2x	1
	Pipelined-GPU, 1 GPU	49.7 s	12.8x	261x	16
	Pipelined-GPU, 2 GPUs	26.6 s	23.9x	487x	16
3 K20s	Pipelined-GPU, 3 GPUs	17 s	37.4x	759x	16

Sequential Implementation

Existing Implementations

ImageJ/Fiji

- Java code
- Multithreaded
- Timing: 3.6 hours!

NIST Prototype

- MATLAB code:
  - Timing: 17.5 min
- Remarks:
  - Caching file reads and FFT results?
  - Multi-threaded FFT routines
  - Optimized or multithreaded code for vector operations?

FFTW 3.3 (fftw.org)

Auto-tuning software

- Create plan to compute FFT
  - Based on CPU properties & FFT dimensions
- Planning mode specifies effort to find "*best*" FFT algorithm

Planning Mode	Planning Time	Execution Time
Estimate	0.02 s	137.7 ms
Measure	4 min 23 s	66.1 ms
Patient	4 min 23 s	66.1 ms
Exhaustive	7 min 1 s	66.1 ms

Amortized planning cost

- Save plan to (re)use later
- Run prior to stitching computation

Optimizations in Seq. Version

Memory I

- Free a tile's transform memory as soon as possible
  - Use reference counts

Memory II

- Traversal order:
  - Chained diagonal
- Maximum memory:
  - Short diagonal + 1
  - Pre-allocate at start & recycle

SSE intrinsics:

- Normalized Cross Correlation factors (step 3)
- Max reduction (step 5)

Results

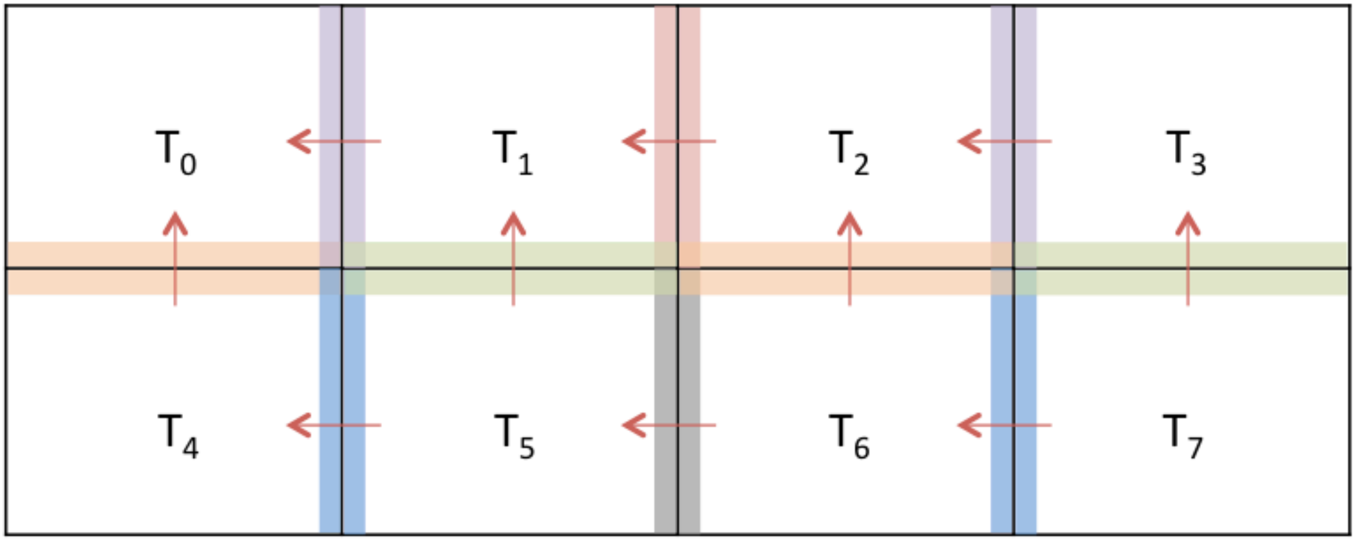
- > 80% of computation in forward and backward Fourier transforms
- Timing: 10.6 min

Speedups

ImageJ/Fiji	21
NIST prototype	1.6

Simple Multi-Threaded Implementation

Simple Multi-Threaded



- 8-way decomposition
- Arrows & shaded areas denote dependencies

- Spatial domain decomposition, one thread per partition
- Handle inter-partition dependencies via *barriers*

Simple Multi-Threaded…

Three phases for all threads separated by barriers:

1. Compute FFT of own images

   Compute relative displacements of tiles with no inter-partition dependencies

   Release memory of transforms w/o dependents

   Barrier

2. Compute relative displacements for remaining tiles (on north & east partition boundaries)

   Barrier

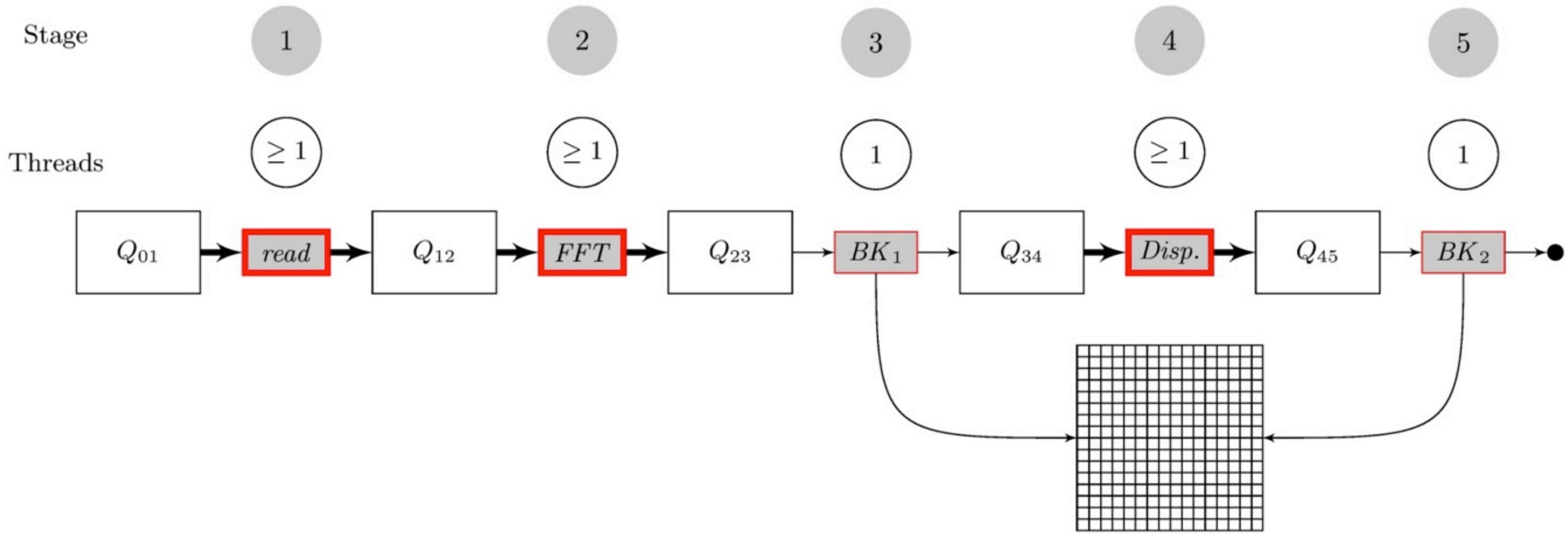
3. Release memory of remaining transforms

Simple Multi-Threaded…

- Timing: 1 min 35 s w/16 threads
    - Used to be 4 min 56 s w/8 threads in "Estimate" planning
- Load imbalance:
    - $T_{0:}$ processes all its tiles in phase 1; idle in phase II
    - T_1–T_7: cannot finish in phase I; different workloads in phase II
    - Unequal partition sizes
- Saturated I/O subsystem
    - Threads concurrently try to read image files
- Hyper-threading
    - Takes advantage of threads with mixed characteristics
    - FFTW functions optimize locality & are CPU-bound

Pipelined Multi-Threaded Implementations

Pipelined Multi-Threaded, v1

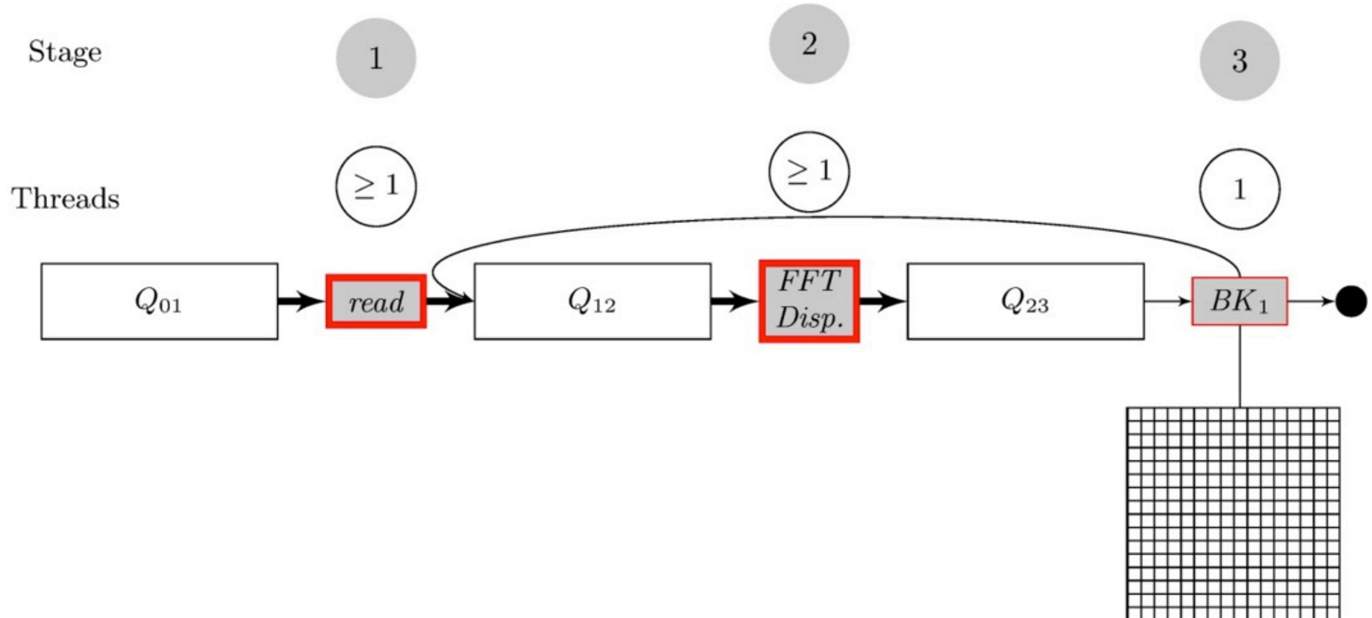


- 5-stage pipeline
  - Producer-consumer pattern
  - Queues with built-in synchronization & size limits
    - Reports max size & logs entries (for debugging)
    - First queue, Q_{01}, is optimized away
  - Memory management restricts number of images in system

Pipelined v1—Details & Optimizations

- 5-stage pipeline
- Producer-consumer pattern
- Queues
  - Built-in synchronization & size limits
    - Synchronization via mutexes & spinlocks
  - Log entries & report max size (for debugging)
- Seq. version optimizations
- Q_{01} optimized away
- Memory management
  - Restrict # images in flight
  - Throttle reader(s)
- Threads
  - 1 reader
  - 2 bookkeepers
  - *n* FFT & 2*n* Rel. Disp.

Pipelined Multi-Threaded, v2



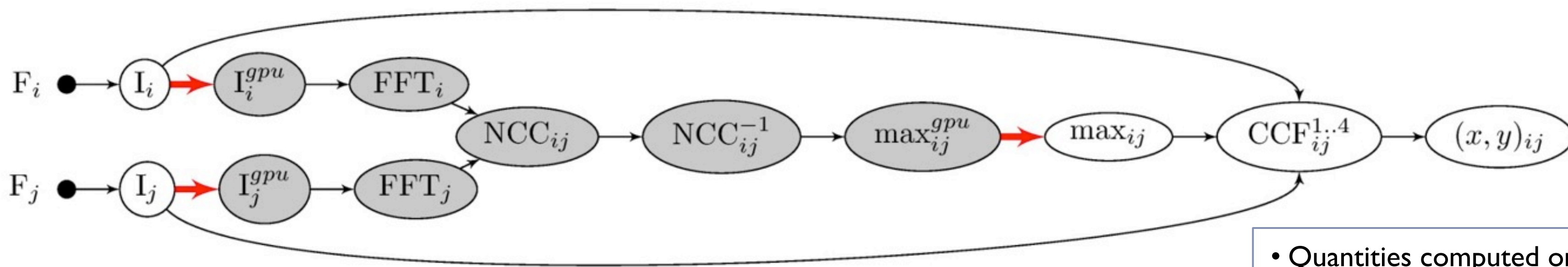
- 3-stage pipeline
  - Based on 5-stage pipeline version
  - Merge work queues into one priority queue
    - Favor relative displacement computation
    - Simpler thread allocation & better thread utilization
  - Merge bookkeeping queues

CPU-Only Speedups

	Time	ImageJ/Fiji	NIST prototype	Sequential
ImageJ/Fiji	3.7 h			
NIST proto.	17.5 min			
Sequential	10.6 min	20.3x	1.65x	1
Simple MT	96 s	135x	10.9x	6.6x
Pipelined MT	84 s	154x	12.5x	7.5x

Simple GPU Implementation

Simple GPU

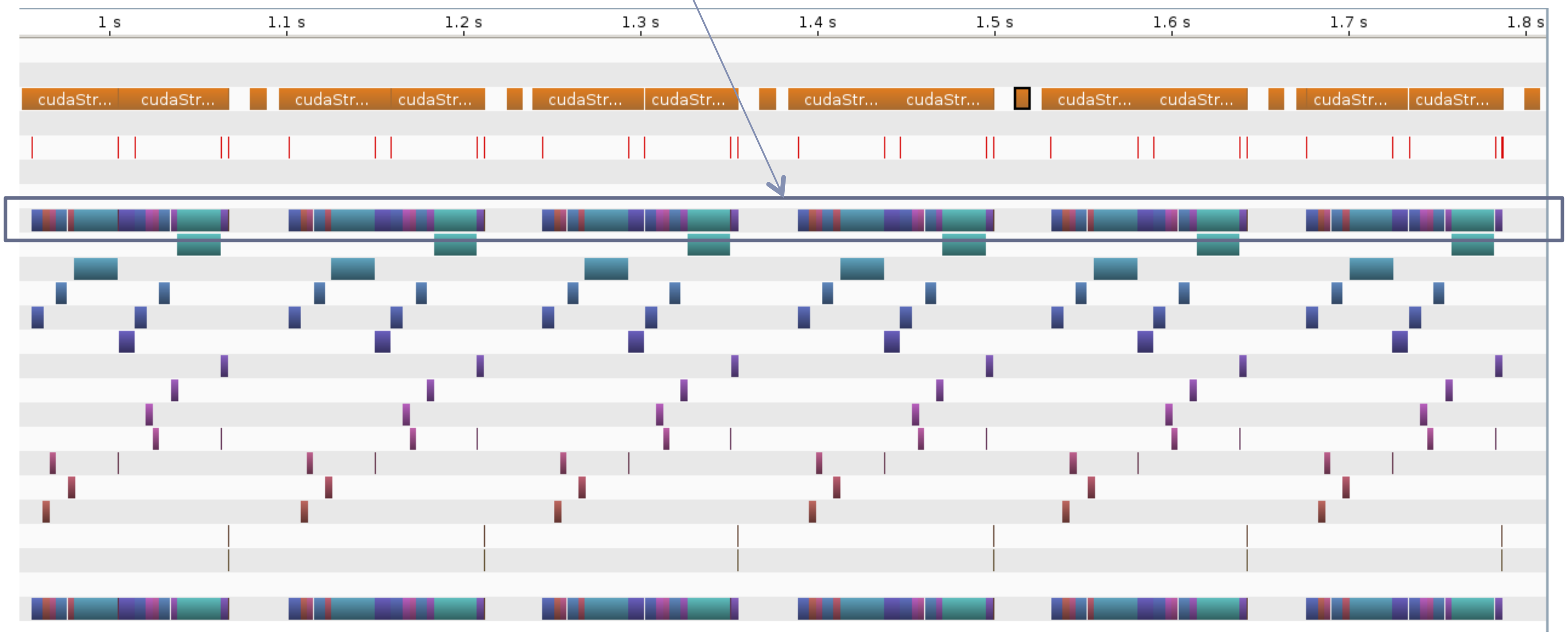


- Quantities computed on GPU appear in gray.
- Red arrows (→): CPU-GPU copy operation.

- Based on sequential implementation
- Offloads most computational tasks to GPU
  - CUFFT function calls for forward & backward transforms
  - Custom CUDA kernels for all other computations
- Copies image data to GPU memory
- Copies results back from GPU memory to RAM

Simple GPU—1 s profile

Single stream
Large repeated gaps



Simple GPU…

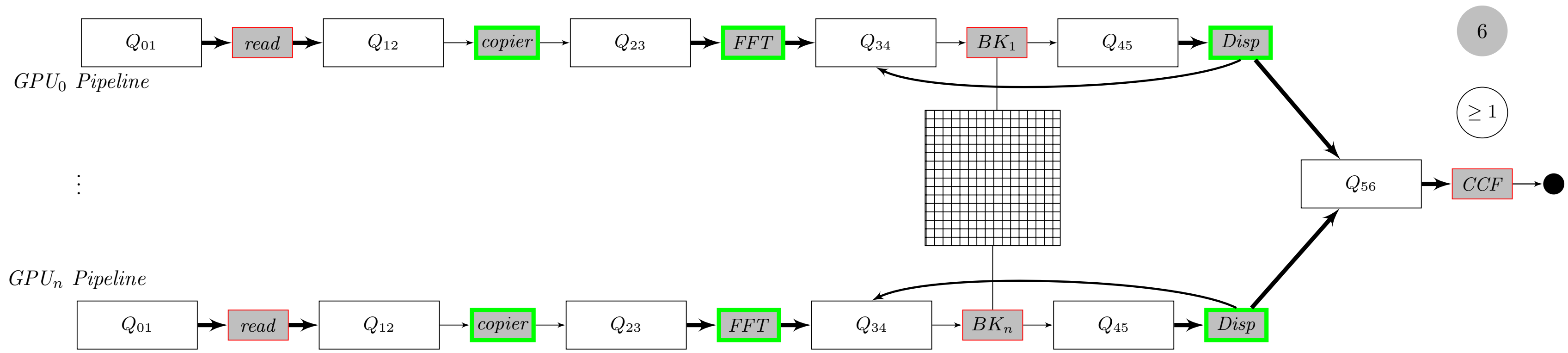
- Timing
  - 9.3 min
  - Speedup 1.14x!

- Optimizations
  - Custom kernels
  - Compute CCFs on CPU

- Conclusion
  - High cost of easy portability!

Pipelined GPU Implementation

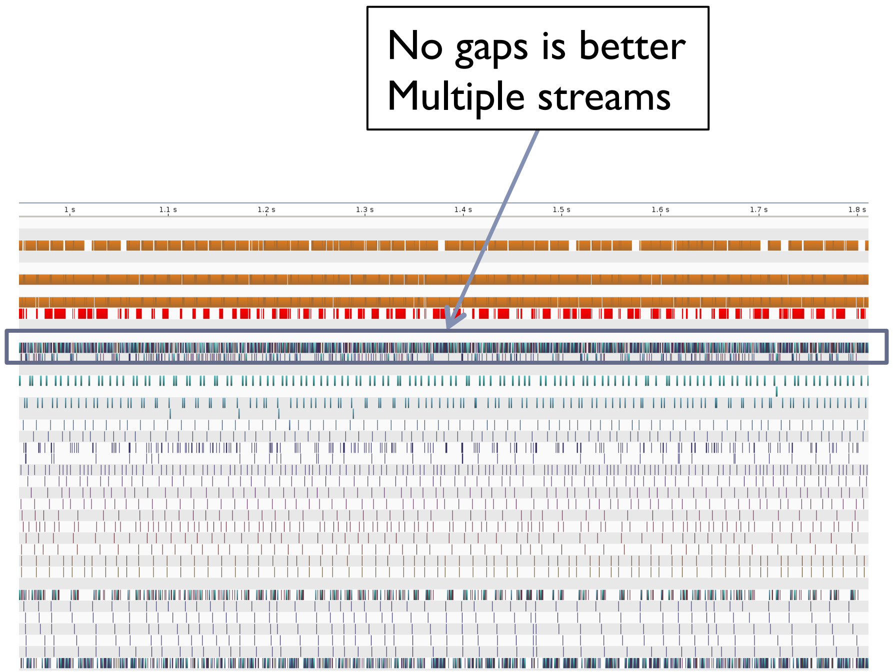
Pipelined GPU



- Seven stage pipeline:
  - Based on pipelined multi-threaded implementation
- CPU threads per GPU:
  - 1 of reader, copier, FFT compute, & rel. displ. compute
  - 2 bookkeepers
- For all GPUs
  - Multiple CPU CCF compute threads

Pipelined GPU—Optimizations

- Asynchronous copy:
  - Overlaps CPU-GPU transfers with tasks on CPU & GPU
- Peer-2-peer copy
  - Between GPUs
- Uses all available resources:
  - Two CPUs
  - Two GPUs
- Keeps GPUs busy



Same 1 s profile as "Simple GPU"

Speedups

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Simple GPU	9.3 min	23.2x	1.79x	1.14x
Pipelined GPU, 1 GPU	49.7 s	261x	21.1x	12.8x
Pipelined GPU, 2 GPUs	26.6 s	487x	39.5x	23.9x

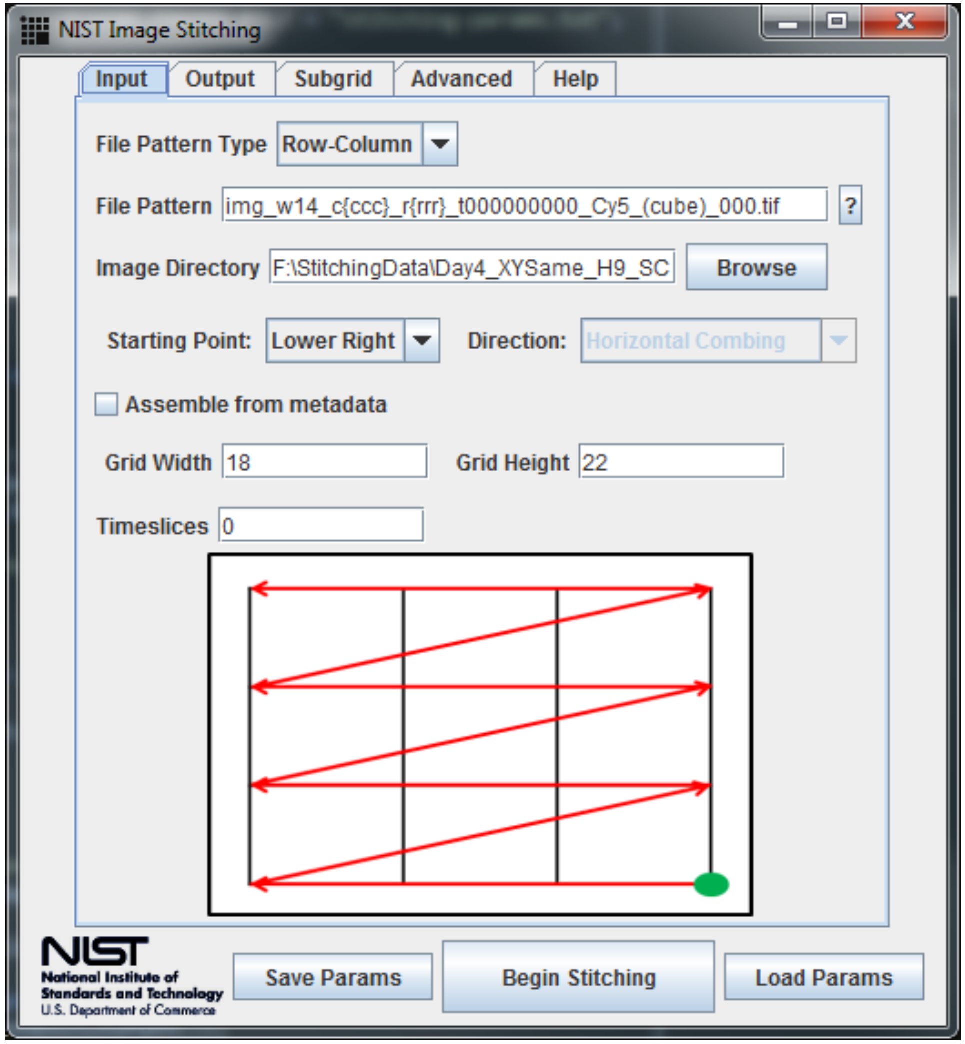
More Recent Results

- IBM Power8 + 3 x NVIDIA K40 GPUs
  - 13 s

Upcoming Code Release

- Java plugin
  - ImageJ/Fiji
  - Stitching + visualization
- Status:
  - Code review + fixes
- Release
  - Q1 2015
- Machine specs
  - Intel Xeon E5-2620 @ 2.3 GHz
    - 6 physical cores (12 logical)
  - 64 GB RAM
  - NVIDIA Tesla C2075
- Java performance
  - CUDA: 134 s
  - FFTW: 203 s
  - Java 32-bit FFT: 99.6 s

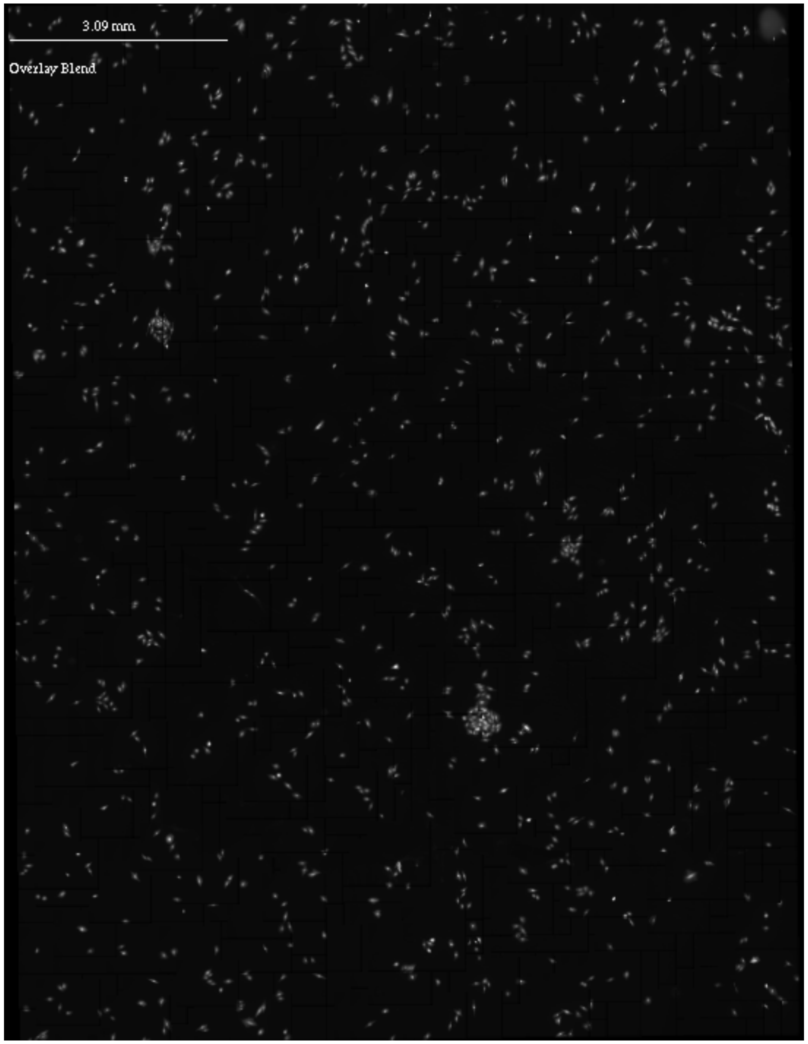
ImageJ Plugin

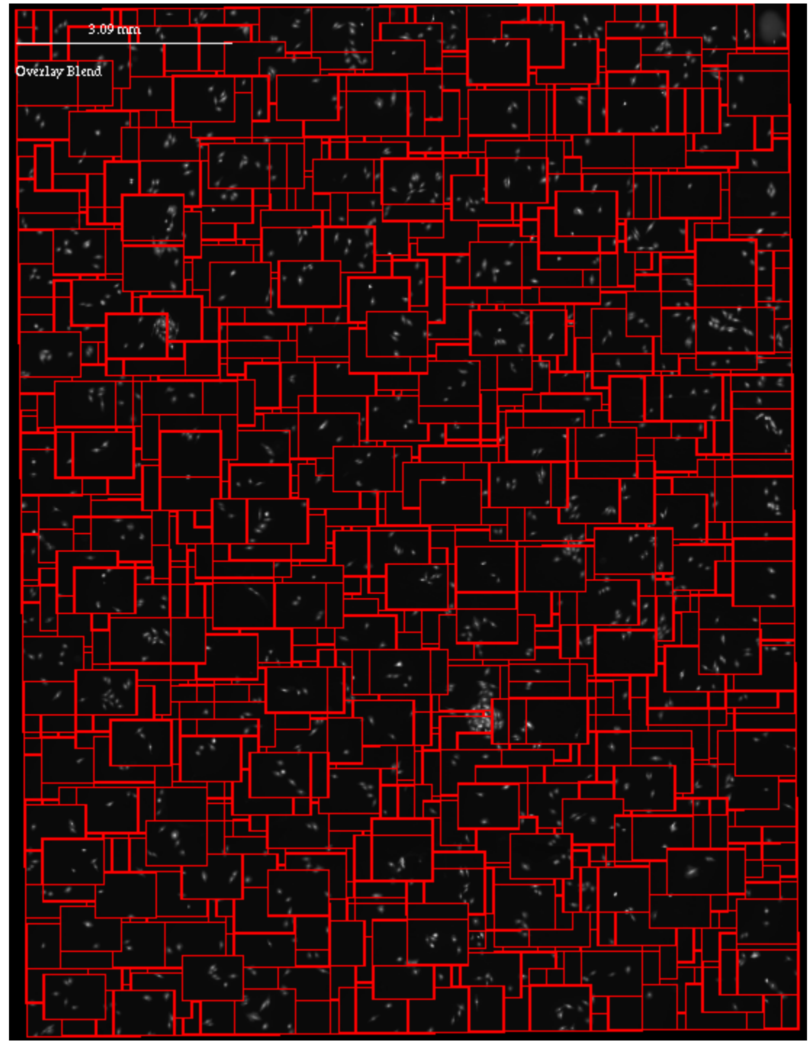


Visualization Overview

- Properties of data
  - Too big to display
  - Impossible to interpret as a whole
  - Sparse regions of interest
- Properties of data access
  - Users
    - Limited capacity for data perception
  - Programs
    - Need pixel-level precision
- Preprocessing
  - Generate and save image pyramids for all tiles
  - Advantage
    - Load minimum data to display given zoom level
- Cache lowest resolution reconstructed image
- Compose partial stitched image on demand

Stitched Images





Lessons Learned

Programs ≠ Algorithms + Data Structures

- Algorithm
  - Mathematical specification of sets of operations
- Data Structures
  - Logical organization of data
- View missing critical aspects for HPC!

Performance & Scalability

- Algorithms + Data Structures = Programs
  - Niklaus Wirth, 1973

- Algorithms + Data Structures + Scheduling + Memory Management = High Performance Programs

Coarse-Grained Parallelism

- Parallel Tasks
  - Decomposition of "Algorithm + Data Structures"
  - Data parallelism for particular operations
- Memory
  - Critical resource to manage
- Data Motion
  - Includes inter-process communication
  - Major delays!
- Schedule
  - Essential to tie together all of the above

Lessons Learned, v 0.2

- It works!
- Understand your computation
  - Correct choice of algorithm
    - $O(n \log n)$ vs. $O(n^2)$ or $O(n)$ vs. $O(n)$
  - Target 90% vs. 10%
- Think asynchronous
- Throw-away code
  - Performance oriented prototypes

Lessons Learned, v 0.2…

- Performance as 1st class citizen
  - Edit-compile-debug → edit-compile-debug-measure
    - Use visualization tools
- Performance vs. portability
- Widely applicable techniques
  - MATLAB prototype: 17 min → ~ 4-5 min
- Java implementation
  - Minutes vs. hours

Lessons Learned, v 0.2…

- Lack of tools
  - Refactoring 10 KLOC (ZENO) feasible by 1-person
  - 100 KLOC beyond scalability limit
- Kernels essentially invariant
  - Image stitching & ZENO
- Performance-oriented tools
  - Instrument code
  - Isolate code sections into kernels
  - Compose kernels into schedules
  - Meter & reuse memory

Closure—General

- 24x speedup (w.r.t. sequential implementation)
  - ~500x w.r.t. ImageJ/Fiji
- Representative data set:
  - 42x59 grid
  - ~ 0.5 minutes
- Low memory footprint by design
  - 4 GB of RAM
- Can budget compute time to:
  - Generate stitched image
  - **Carry out additional analysis**
  - Enables computationally steerable experiments

Closure—CPU & GPU Scalability

- Simple multi-threaded implementation
  - Does not scale well with threads
    - Performance tanks as the number of threads increases past 8
  - Attributed to:
    - Disk I/O being saturated
    - Load Imbalance

- Pipelined implementation
  - Scales well
    - Performance improves as the number of threads increases
    - Takes advantage of multiple GPUs
  - Attributed to:
    - Single reader thread able to keep disk busy without saturation
    - Load is balanced with pool of worker threads

Closure—Additional Work

- ImageJ plug-in + code release
  - Plug-in + ImageJ visualization
  - Visualization tool
  - C++ code
- Integrate into microscope controller software
  - Real-time feedback

Closure—Additional Work

- Systematize approach & analysis into API:
  - Tim's Ph.D. thesis

  - Task graph model
  - Execution pipeline model
    - Mapping between two

  - Memory management
  - Workflow scheduler
  - Petri nets

- Apply to other problems

Closure

- Dramatic performance improvements
  - Often within reach
- Requires software re-design
  - Tool support?
- May be at odds with portability
  - Is portability overvalued?

Questions?