

# Implementing and Tuning Irregular Programs on GPUs

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Computer Science

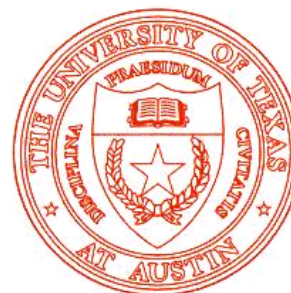
Texas State University-San Marcos



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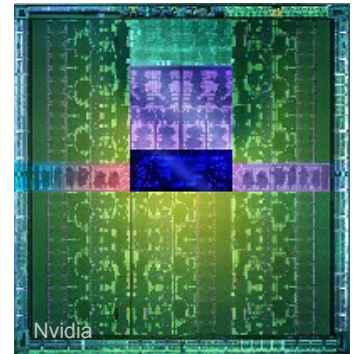
Computational Engineering and Sciences

The University of Texas at Austin



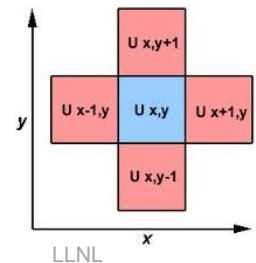
# GPU Advantages over CPUs

- Comparing GTX 680 to Xeon E5-2687W
  - Both released in March 2012
- Peak performance and main-memory bandwidth
  - 8x as many operations executed per second
  - 4x as many bytes transferred per second
- Cost-, energy-, and area-efficiency
  - 29x as much performance per dollar
  - 6x as much performance per watt
  - 11x as much performance per area



# Codes Suitable for GPU Acceleration

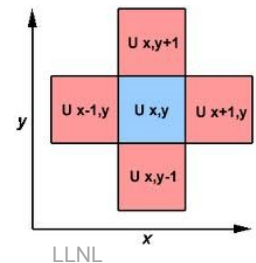
- Clearly, we should be using GPUs all the time
  - So why aren't we?
- GPUs can only accelerate some types of codes
  - Need lots of parallelism, data reuse, and **regularity** (in memory accesses and control flow)
- Mostly **regular** codes have been ported to GPUs
  - E.g., matrix codes executing many ops/word
    - Dense matrix operations (Level 2 and 3 BLAS)
    - Stencil codes (PDE solvers)



# Codes Suitable for GPU Acceleration

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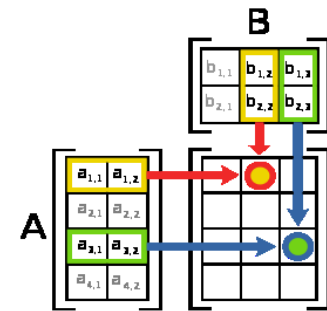
*Our goal is to also handle irregular codes well*



# Regular Programs

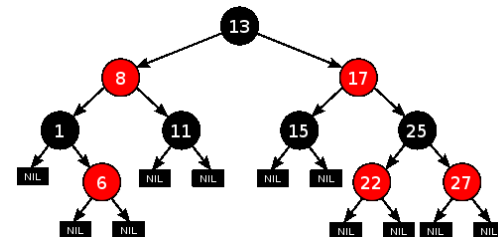
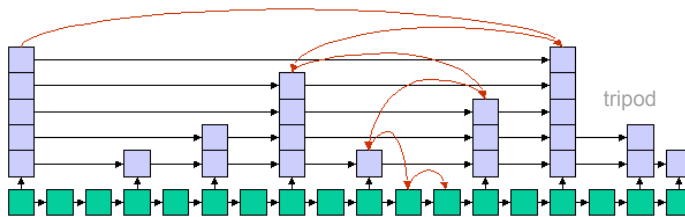
- Typically operate on arrays and matrices
  - Data is processed in fixed-iteration FOR loops
- Have statically **predictable** behavior
  - Exhibit mostly strided memory access patterns
  - Control flow is mainly determined by input *size*
  - Data dependencies are static and not loop carried
- Example

```
for (i = 0; i < size; i++) {  
    c[i] = a[i] + b[i];  
}
```



# Irregular Programs

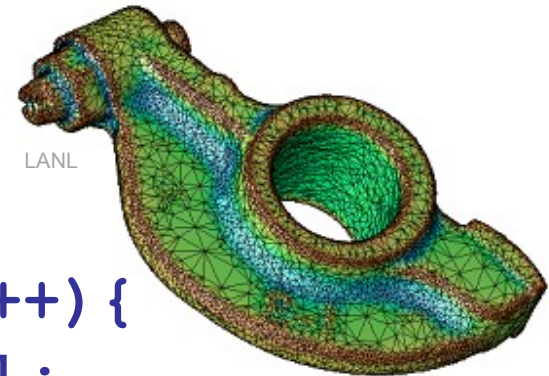
- Are important and widely used
  - Social network analysis, data clustering/partitioning, discrete-event simulation, operations research, meshing, SAT solving,  $n$ -body simulation, *etc.*
- Typically operate on **dynamic** data structures
  - Graphs, trees, linked lists, priority queues, *etc.*
  - Data is processed in variable-iteration WHILE loops



# Irregular Programs (cont.)

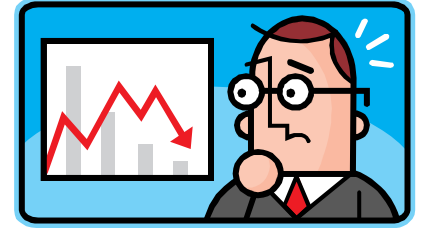
- Have statically **unpredictable** behavior
  - Exhibit pointer-chasing memory access patterns
  - Control flow depends on input *values* and may change
  - Data dependences have to be detected dynamically
- Example

```
while (pos != end) {  
    v = workset[pos++];  
    for (i = 0; i < count[v]; i++) {  
        n = neighbor[index[v] + i];  
        if (process(v,n)) workset[end++] = n;  
    }  
}
```



# GPU Implementation Challenges

- Indirect and irregular memory accesses
  - Little or **no coalescing** [low bandwidth]
- Memory-bound pointer chasing
  - **Little locality** and computation [exposed latency]
- Dynamically changing irregular control flow
  - Thread **divergence** [loss of parallelism]
- Input dependent and changing data parallelism
  - Load **imbalance** [loss of parallelism]

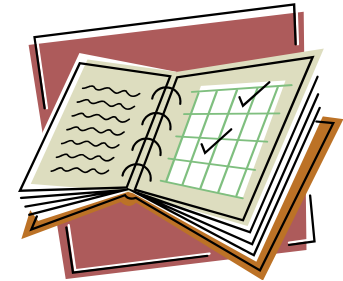


Naïve implementation results in poor performance



# Outline

- Introduction
- Irregular codes and basic optimizations
- Irregular optimizations
- Performance results
- General guidelines
- Summary



# Our Irregular Programs

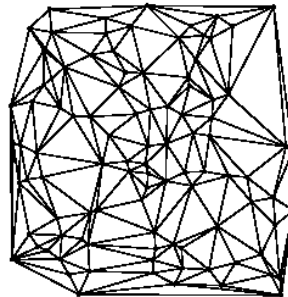
- Mostly taken from **LonestarGPU** benchmark suite
  - Set of currently seven irregular CUDA codes

*<http://iss.ices.utexas.edu/?p=projects/galois/lonestargpu>*

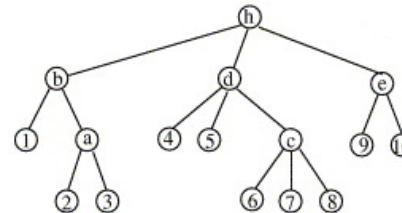
Benchmark	Description	Lines of Code	Number of kernels
BFS	Breadth-first search	275	2
BH	Barnes-Hut $n$ -body simulation	1,069	9
DMR	Delaunay mesh refinement	958	4
MST	Minimum spanning tree	446	8
PTA	Points-to analysis	3,494	40
SP	Survey propagation	445	3
SSSP	Single-source shortest paths	614	2

# Primary Data Structures

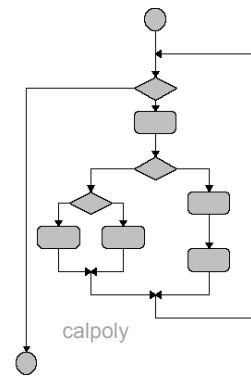
- Road networks
  - BFS, Max-flow, MST, and SSSP
- Triangulated meshes
  - DMR
- Control-flow graphs
  - PTA
- Unbalanced octrees
  - BH
- Bi-partite graphs
  - SP



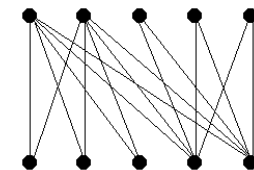
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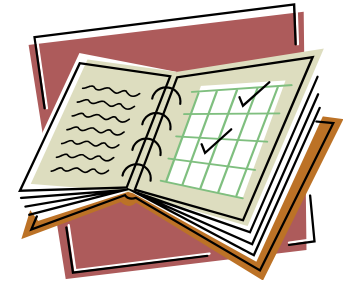
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# Basic CUDA Code Optimizations

- Our codes include many **conventional** optimizations
  - Use structure of arrays, keep data on GPU, improve memory layout, cache data in registers, re-compute instead of re-load values, unroll loops, chunk work, employ persistent threads, and use compiler flags
- Conventional **parallelization** optimizations
  - Use light-weight locking, atomics, and lock-free code; minimize locking, memory fences, and volatile accesses
- Conventional **architectural** optimizations
  - Utilize shared memory, constant memory, streams, thread voting, and rsqrtf; detect compute capability and number of SMs; tune thread count, blocks per SM, launch bounds, and L1 cache/shared-memory configuration

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# Irregular CUDA Code Optimizations

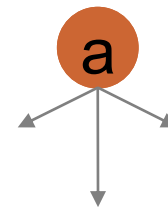
	Category	Optimization	Applications
1	Synchronization	Push versus pull	BFS, PTA, SSSP
		Combined memory fences	BH-summ, BH-tree
		Wait-free pre-pass	BH-summ
2	Memory	Kernel unrolling	BFS, SSSP
		Warp-centric execution	BH-force, PTA
		Computation onto traversal	BH-sort, BH-summ
3	Algorithm	Algorithm choice	Max-flow, SSSP
		Implementation adaptation	MST, SSSP
		Algebraic properties	BFS, SP, SSSP
4	Scheduling	Sorting work	BH-force, DMR, PTA
		Dynamic configuration	DMR, PTA
		Kernel fusion and fission	DMR, MST, SP
		Communication onto computation	BH, PTA

# Push versus Pull

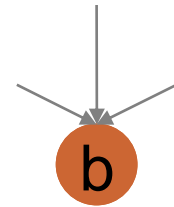
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<b>Synchronization</b>	Push versus pull	BFS, PTA, SSSP
	Combined memory fences	BH-summ, BH-tree
	Wait-free pre-pass	BH-summ

- Information may flow in a push- or pull-based way
  - Push-based data-driven code is **work-efficient**
  - Pull-based code **minimizes synchronization**
- In BFS and SSSP, we use a push-based model
- In PTA, we use a pull-based model
  - Similar to scatter/gather



push-based



pull-based

# Combined Memory Fences

1

<b>Synchronization</b>	Push versus pull	BFS, PTA, SSSP
	Combined memory fences	BH-summ, BH-tree
	Wait-free pre-pass	BH-summ

- Memory fence operations can be slow
  - Combining can help even with some load imbalance
- In BH-tree, the block-threads create subtrees, wait at a **syncthreads**, and install the subtrees
- In BH-summ, the block-threads summarize child info, run a **syncthreads**, then update the parents



# Wait-free Pre-pass

1

<b>Synchronization</b>	Push versus pull	BFS, PTA, SSSP
	Combined memory fences	BH-summ, BH-tree
	Wait-free pre-pass	BH-summ

- Use pre-pass to process ready consumers first
  - Instead of waiting, **skip** over unready consumers
  - Follow up with a ‘waitful’ pass in the end
- BH uses multiple pre-passes in summarization
  - Due to high fan-out of octree, most of work is done in pre-passes, thus **minimizing the waiting** in final pass

# Kernel Unrolling

2

Memory	Kernel unrolling	BFS, SSSP
	Warp-centric execution	BH-force, PTA
	Computation onto traversal	BH-sort, BH-summ

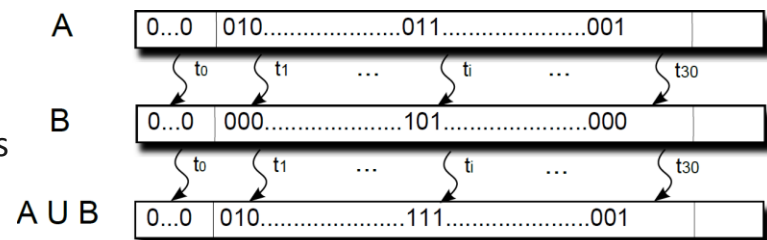
- Kernel unrolling
  - Instead of operating on a single graph element, a thread operates on a (connected) subgraph
  - Improves **locality** and **latency-hiding** ability
  - Helps **propagate** information **faster** through graph
- Useful for memory-bound kernels like BFS & SSSP

# Warp-centric Execution

2

Memory	Kernel unrolling	BFS, SSSP
	Warp-centric execution	BH-force, PTA
	Computation onto traversal	BH-sort, BH-summ

- Forcing warps to stay synchronized in irreg code
  - Eliminates **divergence** and enables **coalescing**
- BH traverses entire warp's **union** of tree prefixes
  - Divergence-free traversal & only need per-warp data
- PTA uses lists with **32 words** per element
  - Enables fast set union & fully coalesced data accesses



# Computation onto Traversal

2

Memory	Kernel unrolling	BFS, SSSP
	Warp-centric execution	BH-force, PTA
	Computation onto traversal	BH-sort, BH-summ

- **Combines multiple passes** over data structure
- In BH-sort, top-down traversal sorts bodies and moves non-null children to front of child-array
- In BH-summ, bottom-up traversal computes center of gravity and counts number of bodies in subtrees

# Algorithm Choice

3

Algorithmic	Algorithm choice	Max-flow, SSSP
	Implementation adaptation	MST, SSSP
	Algebraic properties	BFS, SP, SSSP

- Best algorithm choice is **architecture dependent**
- For Max-flow, push-relabel algorithm is better for CPUs whereas MPM works better on GPUs
- For SSSP, Bellman-Ford algorithm is preferential on GPUs whereas Dijkstra's algorithm yields better serial performance on CPUs

# Implementation Adaptation

3

Algorithmic	Algorithm choice	Max-flow, SSSP
	Implementation adaptation	MST, SSSP
	Algebraic properties	BFS, SP, SSSP

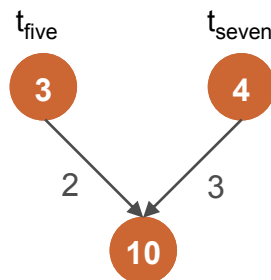
- Implementation may have to be adjusted for GPU
  - **Array-based** graph representations
  - **Topology-** instead of data-driven implementation
- For MST, do not explicitly contract edges
  - Keep graph static and record which nodes are merged
- For SSSP, use topology-driven implementation
  - Avoided synchronization outweighs work inefficiency

# Algebraic Properties

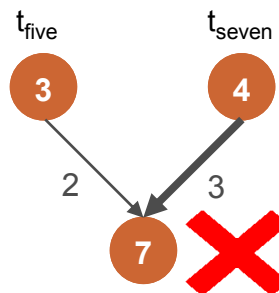
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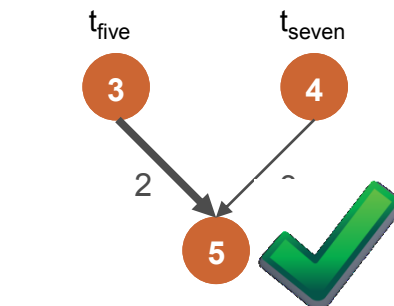
- Exploiting monotonicity property
  - Enables **atomic-free** topology-driven implementation
- In BFS and SSSP, the node distances decrease monotonically; in SP, the product of probabilities



Atomic-free update



Lost-update problem



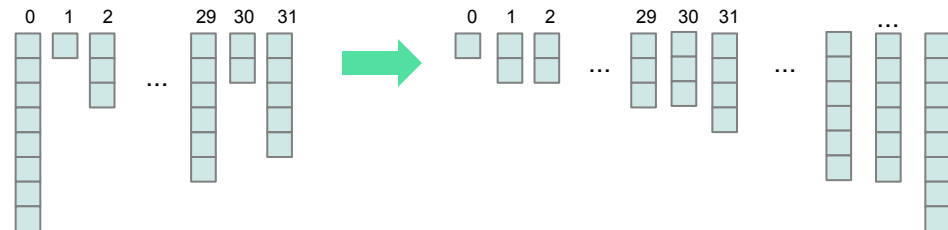
Correction by topology-driven processing,  
exploiting monotonicity

# Sorting Work

4

Scheduling	Sorting work	BH-force, DMR, PTA
	Dynamic configuration	DMR, PTA
	Kernel fusion and fission	DMR, MST, SP
	Communication onto computation	BH, PTA

- Each warp-thread should do similar work
  - Sorting **minimizes divergence** and load **imbalance**
- In BH, bodies are sorted by spatial location; in DMR, triangles are sorted by badness; in PTA, nodes are sorted by in-degrees



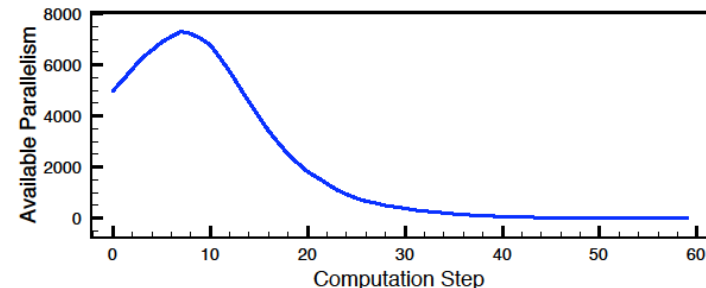


# Dynamic Configuration

4

<b>Scheduling</b>	Sorting work	BH-force, DMR, PTA
	Dynamic configuration	DMR, PTA
	Kernel fusion and fission	DMR, MST, SP
	Communication onto computation	BH, PTA

- Computation should follow **parallelism profile**
  - Fewer threads = fewer conflicts & less sync overhead
- In DMR, the number of **aborts** due to conflicts reduces from 60% and 35% in the first two iterations to 1% and 4.4%
- PTA is similar



# Kernel Fusion and Fission

4

<b>Scheduling</b>	Sorting work	BH-force, DMR, PTA
	Dynamic configuration	DMR, PTA
	Kernel fusion and fission	DMR, MST, SP
	Communication onto computation	BH, PTA

- Kernel fusion
  - **Fast data-sharing** and reduced invocation overhead
- Kernel fission
  - Enables **individually tuned** kernel configurations
- DMR uses fusion to transfer connectivity info
- MST uses fission for various computations

# Communication onto Computation

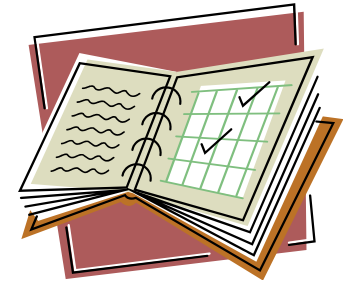
4

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- **Overlap CPU/GPU transfer** with GPU computation
- In BH, the bodies' positions can be sent to the CPU while the next time step starts running
- In PTA, points-to information is incrementally copied to the CPU while the GPU is computing more points-to information

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# Experimental Methodology

- **Quadro 6000** GPU, 1.45 GHz, 6 GB, 448 PEs
- nvcc compiler v4.2 with -arch=sm\_20 -O3 flags
- LonestarGPU program inputs
  - BFS, Max-flow, MST, SSSP: road networks, RMAT graphs, and random graphs
  - BH: random star clusters based on Plummer model
  - DMR: randomly generated 2D meshes
  - PTA: constraint graphs from open-source C/C++ progs
  - SP: randomly generated hard 3-SAT formulae
- Base case: ported optimized multi-core CPU code
- **Best case: includes applicable irreg. optimizations**

# Overall Speedup over Naïve Porting

Benchmark	Input	Speedup
BFS	RMAT20	75.3
	USA	72.8
BH	1M	16.0
	5M	17.9
DMR	1M	55.1
	10M	74.4
MST	RMAT20	1.0
	USA	14.4
PTA	vim	1.1
	tshark	1.5
SP	1M	5.5
	4M	5.5
SSSP	RMAT20	297.4
	USA	196.8

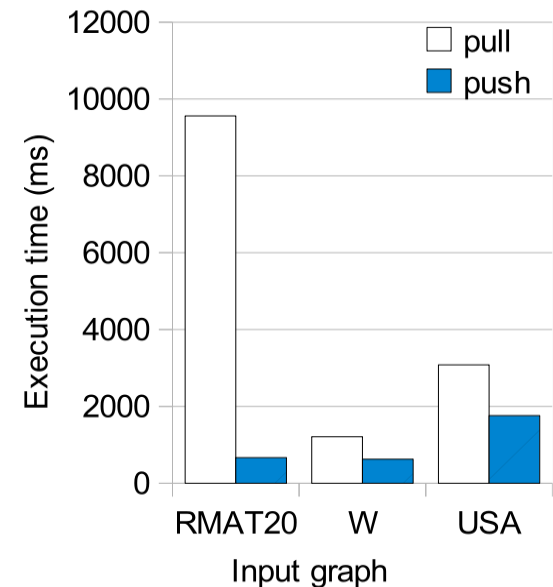
- Irregular optimizations can be **essential**
  - Performance improves by up to 2 orders of magnitude

# Push versus Pull

1

Synchronization	Push versus pull	BFS, PTA, SSSP
	Combined memory fences	BH-summ, BH-tree
	Wait-free pre-pass	BH-summ

- SSSP on various graphs
  - Push (scatter) is better since it propagates info faster
  - Benefit is higher for denser RMAT graph
  - Both the push and pull codes are atomic-free

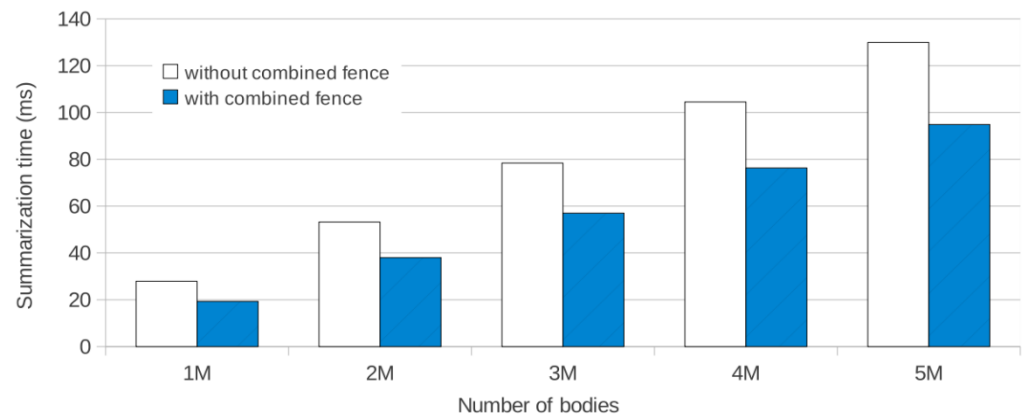


# Combined Memory Fences

1

<b>Synchronization</b>	Push versus pull	BFS, PTA, SSSP
	Combined memory fences	BH-summ, BH-tree
	Wait-free pre-pass	BH-summ

- BH octree building on star clusters
  - Combining multiple memory fences into a single syncthreads
  - 37% to 44% faster despite barrier-induced waiting



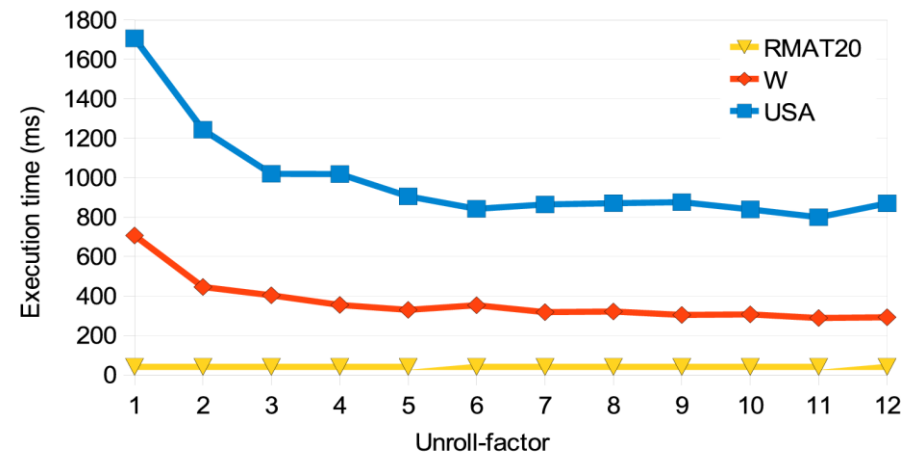


# Kernel Unrolling

2

Memory	Kernel unrolling	BFS, SSSP
	Warp-centric execution	BH-force, PTA
	Computation onto traversal	BH-sort, BH-summ

- SSSP on various graphs
  - Increasing unroll factor improves computation-to-latency ratio
  - Almost halves running time for road networks

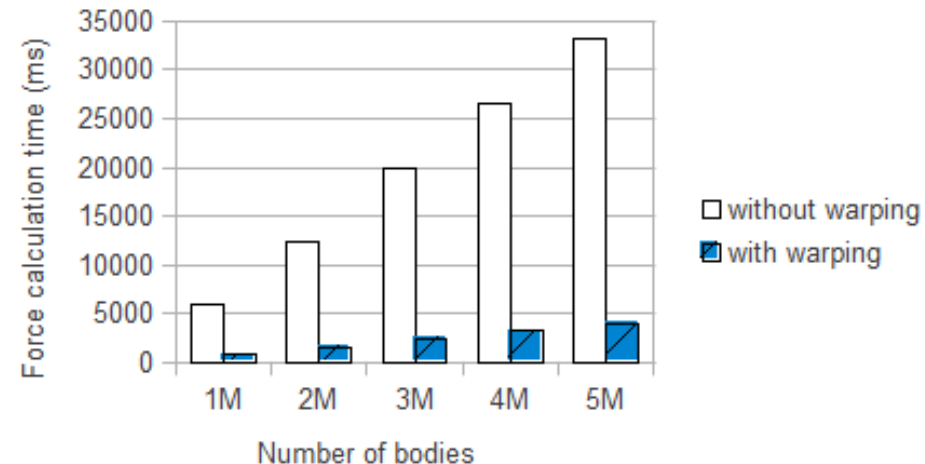


# Warp-centric Execution

2

Memory	Kernel unrolling	BFS, SSSP
	Warp-centric execution	BH-force, PTA
	Computation onto traversal	BH-sort, BH-summ

- BH force calculation on star clusters
  - Warp-based execution enables coalescing and iteration-stack sharing
  - About 8x speedup

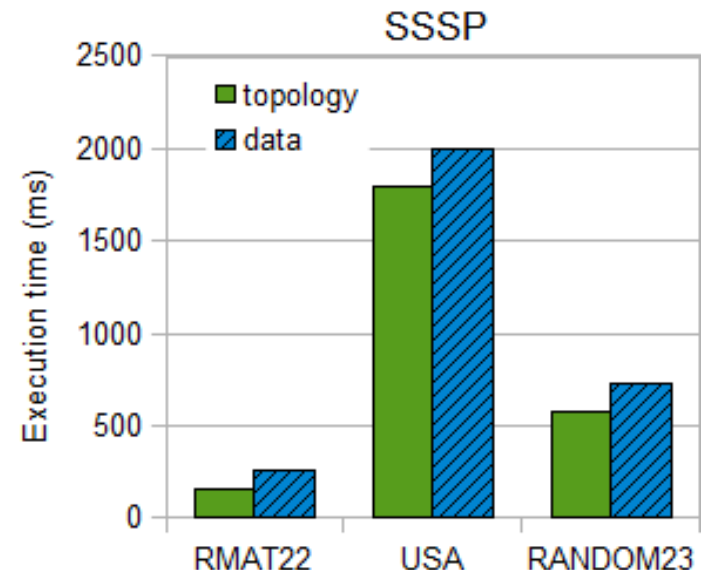


# Implementation Adaptation

3

Algorithmic	Algorithm choice	Max-flow, SSSP
	Implementation adaptation	MST, SSSP
	Algebraic properties	BFS, SP, SSSP

- SSSP on various graphs
  - Work inefficient topology-driven implementation
  - Enables synchronization-free implementation
  - Outperforms data-driven

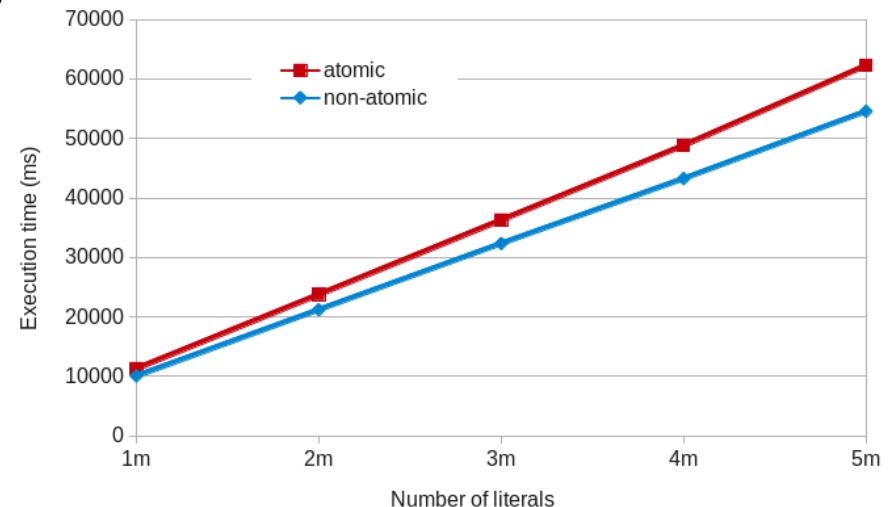


# Algebraic Properties

3

<b>Algorithmic</b>	Algorithm choice	Max-flow, SSSP
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- SP for hard 3-SAT inputs
  - Exploits monotonicity to avoid atomics
  - Performance benefit increases for larger problem sizes

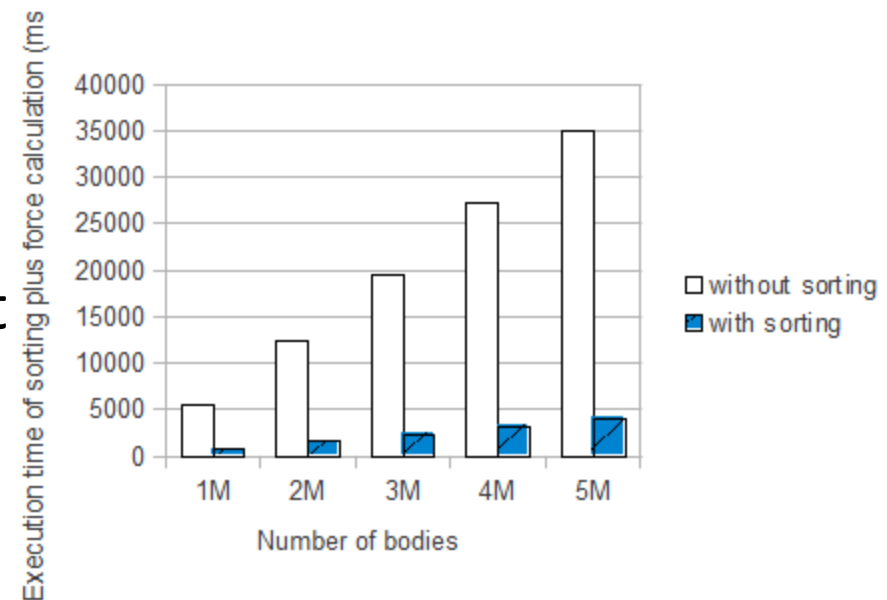


# Sorting Work

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	Dynamic configuration	DMR, PTA
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- BH force calculation and sorting on star clusters
  - Sorting reduces size of union of tree prefixes that warp threads traverse
  - 7.4x to 8.7x speedup

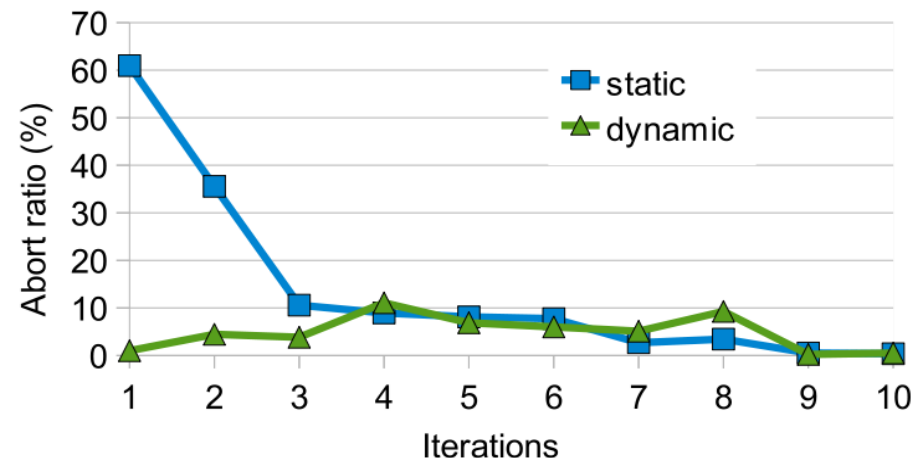


# Dynamic Configuration

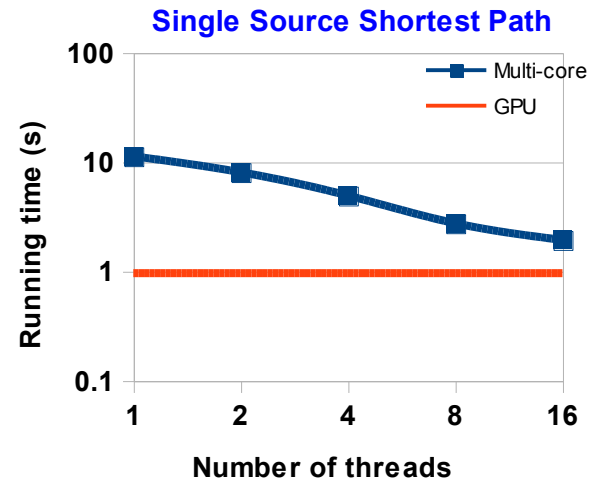
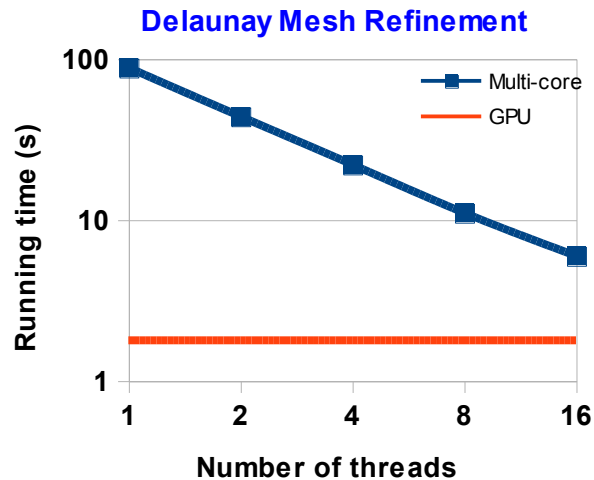
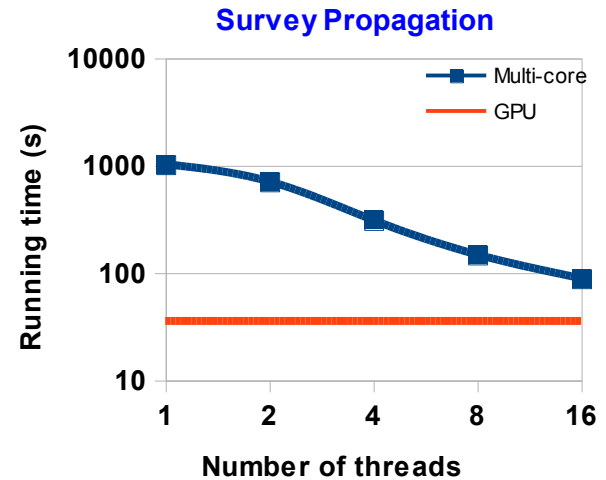
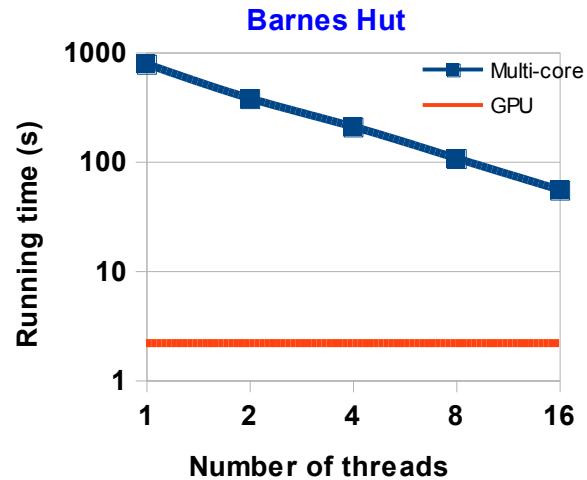
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- DMR on random mesh
  - Dynamic kernel configuration lowers abort ratio from 60% to 1% in first iteration
  - Overall performance improves by 14%



# GPU/CPU Performance Comparison



Inputs: BH : 5M stars (Plummer model), 1 time step  
DMR : 10M triangles, 4.7M bad triangles

SP : 1M literals, 4.2M clauses  
SSSP : 23M nodes, 57M edges

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# CPU/GPU Implementation Differences

- Irregular **CPU** code
  - Dynamically (incrementally) allocated data structure
  - Structure-based data structures
  - Logical lock-based implementation
  - Global/local worklists
  - Recursive or iterative implementation
- Irregular **GPU** code
  - Statically (wholly) allocated data structure
  - Multiple-array-based data structures
  - Lock-free implementation
  - Local or no worklists
  - Iterative implementation

# Exploit Irregularity-friendly Features

- **Massive multithreading**
  - Ideal for hiding latency of irregular mem. accesses
- **Wide parallelism**
  - Great for exploiting large amounts of parallelism
- **Shared memory**
  - Useful for local worklists
  - Fast data sharing
- **Fast thread startup**
  - Essential when launching thousands of threads
- **HW support for reduction and synchronization**
  - Makes otherwise costly operations very fast
- **Lockstep execution**
  - Can share data without explicit synchronization
  - Allows to consolidate iteration stacks
- **Coalesced accesses**
  - Access combining is useful in irregular codes

# Traits of Efficient Irregular GPU Codes

- **Mandatory**
  - Need vast amounts of data parallelism
  - Can do large chunks of computation on GPU
- **Very Important**
  - Cautious implementation
  - DS can be expressed through fixed arrays
  - Uses local (or implicit) worklists that can be statically populated
- **Important**
  - Scheduling is independent of previous activities
  - Easy to sort activities by similarity (if needed)
- **Beneficial**
  - Easy to express iteratively
  - Has statically known range of neighborhoods
  - DS size (or bound) can be determined based on input

# Mandatory Traits

- Need vast amounts of **data parallelism**
  - Small inputs are not worth running on the GPU
  - Many ordered algorithms do not qualify
- Can do **large chunks** of computation on GPU
  - Time-intensive parts of algorithm must run on GPU
  - Avoids frequent CPU-GPU memory transfers



# Very Important Traits

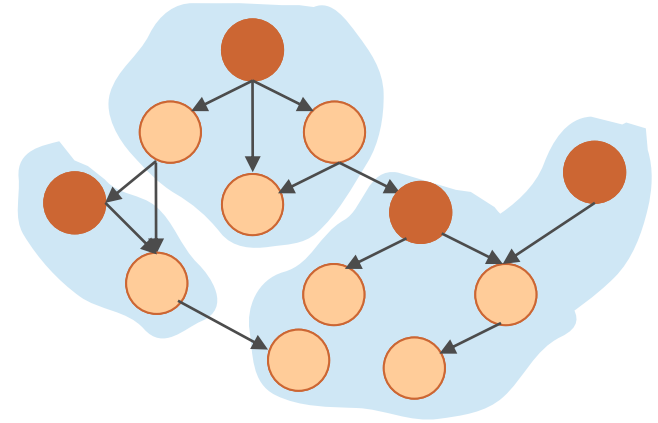
- **Cautious** implementation
  - No rollback mechanism is needed to handle conflicts
- Data struct can be expressed through **fixed arrays**
  - Avoids slow dynamic memory allocation
  - Guarantees contiguous memory
- Uses **local** (or implicit) **worklists** that can be statically populated
  - Avoids serialization point
  - Enables lock-free implementation

# Important Traits

- **Scheduling** is **independent** of or can ignore previous activities
  - Unordered: all nodes active (once or always) or many nodes active (and easy to determine whether active)
  - Ordered: ordered by level, assigned to worklist in 'correct' order, poll until ready
- Easy to **approximately sort** activities by similarity
  - Reduces divergence and enables other optimizations

# Beneficial Traits

- Easy to express **iteratively**
  - Recursion is not well supported
- Has statically known range of **neighborhoods**
  - Enables certain performance optimizations
- Data structure **size** (or upper bound) can be determined based on input
  - Allows one-time fixed allocation or over-allocation



# Outline

- Introduction
- Irregular codes and basic optimizations
- Irregular optimizations
- Performance results
- General guidelines
- **Summary**





# Summary of Optimization Principles

	Category	Optimization	Applications
1	Synchronization	Push versus pull	BFS, PTA, SSSP
		Combined memory fences	BH-summ, BH-tree
		Wait-free pre-pass	BH-summ
2	Memory	Kernel unrolling	BFS, SSSP
		Warp-centric execution	BH-force, PTA
		Computation onto traversal	BH-sort, BH-summ
3	Algorithm	Algorithm choice	Max-flow, SSSP
		Implementation adaptation	MST, SSSP
		Algebraic properties	BFS, SP, SSSP
4	Scheduling	Sorting work	BH-force, DMR, PTA
		Dynamic configuration	DMR, PTA
		Kernel fusion and fission	DMR, MST, SP
		Communication onto computation	BH, PTA

# Summary and Conclusion

- Presented 13 general optimization principles for efficiently implementing irregular GPU codes
  - Necessary because irregular algorithms can be very challenging to accelerate using GPUs
- Today's GPUs can deliver high performance on many irregular codes and can accelerate them
- Code for GPU, do not merely adjust CPU code
  - Requires different data and code structures
  - Benefits from different optimizations



# Further Reading on our Project

- GPU Optimization Principles for Irregular Programs, **submitted**
- Data-driven vs. Topology-driven Irregular Algorithms on GPUs, **IPDPS 2013**
- Atomic-free Irregular Computations on GPUs, **GPGPU 2013**
- Morph Algorithms on GPUs, **PPoPP 2013**
- A Quantitative Study of Irregular Programs on GPUs, **IISWC 2012**
- A GPU Implementation of Inclusion-based Points-to Analysis, **PPoPP 2012**
- An Efficient CUDA Implementation of the Tree-based Barnes-Hut n-Body Algorithm, **GPU Computing Gems 2011**

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