Software Design for PDEs on GPUs

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High Performance Computing and Emerging Architectures
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Collaborators

Chicago Automated Scientific Computing Group:

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  - Dept. of Computer Science, University of Chicago
  - Dept. of Mathematics, University of Chicago

- Peter Brune, (biological DFT)
  - Dept. of Computer Science, University of Chicago

- Dr. Andy Terrel, (Rheagen)
  - Dept. of Computer Science and TACC, University of Texas at Austin
The **PetFMM team:**

- **Prof. Lorena Barba**
  - Dept. of Mechanical Engineering, Boston University

- **Dr. Felipe Cruz**, developer of GPU extension
  - Nagasaki Advanced Computing Center, Nagasaki University

- **Dr. Rio Yokota**, developer of 3D extension
  - Dept. of Mechanical Engineering, Boston University
Collaborators

The **PyLith** Team:

- **Dr. Brad Aagaard** *(PyLith)*
  - United States Geological Survey, Menlo Park, CA

- **Dr. Charles Williams** *(PyLith)*
  - GNS Science, Wellington, NZ
To be widely accepted, GPU computing must be transparent to the user, and reuse existing infrastructure.
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Lessons from Clusters and MPPs

Failure

- Parallelizing Compilers
- Automatic program decomposition

Success

- MPI (Library Approach)
- PETSc (Parallel Linear Algebra)
- User provides only the mathematical description
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Success
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Outline

1. PETSc-GPU
2. FEM-GPU
3. FMM-GPU
**Thrust** is a CUDA library of parallel algorithms

- Interface similar to C++ Standard Template Library
- Containers (*vector*) on both host and device
- Algorithms: *sort, reduce, scan*
- Freely available, part of PETSc configure (*-with-thrust-dir*)
- Included as part of CUDA 4.0 installation
**Cusp** is a CUDA library for sparse linear algebra and graph computations

- Builds on data structures in Thrust
- Provides sparse matrices in several formats (CSR, Hybrid)
- Includes some preliminary preconditioners (Jacobi, SA-AMG)
- Freely available, part of PETSc configure (`-with-cusp-dir`)
VECCUDA

Strategy: Define a new Vec implementation

- Uses Thrust for data storage and operations on GPU
- Supports full PETSc Vec interface
- Inherits PETSc scalar type
- Can be activated at runtime, -vec_type cuda
- PETSc provides memory coherence mechanism
PETSc Objects now hold a coherence flag

<table>
<thead>
<tr>
<th>Flag</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PETSC_CUDA_UNALLOCATED</td>
<td>No allocation on the GPU</td>
</tr>
<tr>
<td>PETSC_CUDA_GPU</td>
<td>Values on GPU are current</td>
</tr>
<tr>
<td>PETSC_CUDA_CPU</td>
<td>Values on CPU are current</td>
</tr>
<tr>
<td>PETSC_CUDA_BOTH</td>
<td>Values on both are current</td>
</tr>
</tbody>
</table>

**Table:** Flags used to indicate the memory state of a PETSc CUDA Vec object.
Also define new **Mat** implementations

- Uses **Cusp** for data storage and operations on GPU
- Supports full PETSc **Mat** interface, some ops on CPU
- Can be activated at runtime, `-mat_type aijcuda`
- Notice that parallel matvec necessitates off-GPU data transfer
Solvers come for Free
Preliminary Implementation of PETSc Using GPU,
Minden, Smith, Knepley, 2010

- All linear algebra types work with solvers
- Entire solve can take place on the GPU
  - Only communicate scalars back to CPU
- GPU communication cost could be amortized over several solves
- Preconditioners are a problem
  - Cusp has a promising AMG
PETSc only needs

# Turn on CUDA
--with-cuda
# Specify the CUDA compiler
--with-cudac='nvcc -m64'
# Indicate the location of packages
# --download-* will also work soon
--with-thrust-dir=/PETSc3/multicore/thrust
--with-cusp-dir=/PETSc3/multicore/cusp
# Can also use double precision
--with-precision=single
Example
Driven Cavity Velocity-Vorticity with Multigrid

```
ex50 -da_vec_type seqcusp
   -da_mat_type aijcusp -mat_no_inode # Setup types
   -da_grid_x 100 -da_grid_y 100 # Set grid size
   -pc_type none -pc_mg_levels 1 # Setup solver
   -preload off -cuda_synchronize # Setup run
   -log_summary
```

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PDE on GPU
IMA '10 15 / 57
Outline

1. PETSc-GPU
2. FEM-GPU
   - Analytic Flexibility
   - Computational Flexibility
   - Efficiency
3. FMM-GPU
Low Order FEM on GPUs

- Analytic Flexibility
- Computational Flexibility
- Efficiency

http://www.bitbucket.org/aterrel/flamefem
What are the Benefits for current PDE Code?

Low Order FEM on GPUs

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2 FEM-GPU
- Analytic Flexibility
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Analytic Flexibility

Laplacian

\[ \int_T \nabla \phi_i(x) \cdot \nabla \phi_j(x) dx \]  

(1)

element = FiniteElement('Lagrange', tetrahedron, 1)
v = TestFunction(element)
u = TrialFunction(element)
a = inner(grad(v), grad(u)) * dx
\[ \int_{\mathcal{T}} \nabla \phi_i(x) \cdot \nabla \phi_j(x) \, dx \] (1)

```python
element = FiniteElement('Lagrange', tetrahedron, 1)
v = TestFunction(element)
u = TrialFunction(element)
a = inner(grad(v), grad(u)) * dx
```
\[ \frac{1}{4} \int_{T} \left( \nabla \vec{\phi}_i(x) + \nabla^T \vec{\phi}_i(x) \right) : \left( \nabla \vec{\phi}_j(x) + \nabla^T \vec{\phi}_j(x) \right) \, dx \quad (2) \]

element = VectorElement('Lagrange', tetrahedron, 1)
v = TestFunction(element)
u = TrialFunction(element)
a = inner(sym(grad(v)), sym(grad(u)))*dx
\[
\frac{1}{4} \int_T \left( \nabla \phi_i(x) + \nabla^T \phi_i(x) \right) : \left( \nabla \phi_j(x) + \nabla^T \phi_j(x) \right) \, dx
\] (2)

\begin{verbatim}
  element = VectorElement('Lagrange', tetrahedron, 1)
  v = TestFunction(element)
  u = TrialFunction(element)
  a = inner(sym(grad(v)), sym(grad(u))) * dx
\end{verbatim}
\[
\frac{1}{4} \int_T \left( \nabla \vec{\phi}_i(\mathbf{x}) + \nabla^T \vec{\phi}_i(\mathbf{x}) \right) : C : \left( \nabla \vec{\phi}_j(\mathbf{x}) + \nabla^T \vec{\phi}_j(\mathbf{x}) \right) d\mathbf{x} \quad (3)
\]

```python
element = VectorElement('Lagrange', tetrahedron, 1)
cElement = TensorElement('Lagrange', tetrahedron, 1,
(dim, dim, dim, dim))
v = TestFunction(element)
u = TrialFunction(element)
C = Coefficient(cElement)
i, j, k, l = indices(4)
a = sym(grad(v))[i,j]*C[i,j,k,l]*sym(grad(u))[k,l]*dx
```

Currently broken in FEniCS release
\[
\frac{1}{4} \int_{\mathcal{T}} \left( \nabla \vec{\phi}_i(\mathbf{x}) + \nabla^T \vec{\phi}_i(\mathbf{x}) \right) : C : \left( \nabla \vec{\phi}_j(\mathbf{x}) + \nabla^T \vec{\phi}_j(\mathbf{x}) \right) \, d\mathbf{x}
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element = VectorElement('Lagrange', tetrahedron, 1)
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Currently **broken** in FEniCS release
Outline

2. FEM-GPU
   - Analytic Flexibility
   - Computational Flexibility
   - Efficiency
Form Decomposition

Element integrals are decomposed into analytic and geometric parts:

\[
\int_{\mathcal{T}} \nabla \phi_i(\mathbf{x}) \cdot \nabla \phi_j(\mathbf{x}) d\mathbf{x} = \int_{\mathcal{T}} \frac{\partial \phi_i(\mathbf{x})}{\partial x_\alpha} \frac{\partial \phi_j(\mathbf{x})}{\partial x_\alpha} d\mathbf{x}
\]

(4)

\[
= \int_{\mathcal{T}_{\text{ref}}} \frac{\partial \xi_\beta}{\partial x_\alpha} \frac{\partial \phi_i(\xi)}{\partial \xi_\beta} \frac{\partial \xi_\gamma}{\partial x_\alpha} \frac{\partial \phi_j(\xi)}{\partial \xi_\gamma} |J| d\xi
\]

(5)

\[
= \frac{\partial \xi_\beta}{\partial x_\alpha} \frac{\partial \xi_\gamma}{\partial x_\alpha} |J| \int_{\mathcal{T}_{\text{ref}}} \frac{\partial \phi_i(\xi)}{\partial \xi_\beta} \frac{\partial \phi_j(\xi)}{\partial \xi_\gamma} d\xi
\]

(6)

\[
= G^{\beta \gamma}(\mathcal{T}) K_{\beta \gamma}^{ij}
\]

(8)

Coefficients are also put into the geometric part.
Form Decomposition

Additional fields give rise to **multilinear** forms.

\[
\int_{\mathcal{T}} \phi_i(x) \cdot (\phi_k(x) \nabla \phi_j(x)) \, dA
\]

\[
= \int_{\mathcal{T}} \phi_i^\beta(x) \left( \phi_k^\alpha(x) \frac{\partial \phi_j^\beta(x)}{\partial x_\alpha} \right) \, dA
\]

\[
= \int_{\mathcal{T}_{\text{ref}}} \phi_i^\beta(\xi) \phi_k^\alpha(\xi) \frac{\partial \xi_\gamma}{\partial x_\alpha} \frac{\partial \phi_j^\beta(\xi)}{\partial \xi_\gamma} |J| \, dA
\]

\[
= \frac{\partial \xi_\gamma}{\partial x_\alpha} |J| \int_{\mathcal{T}_{\text{ref}}} \phi_i^\beta(\xi) \phi_k^\alpha(\xi) \frac{\partial \phi_j^\beta(\xi)}{\partial \xi_\gamma} \, dA
\]

\[
= G^{\alpha\gamma}(\mathcal{T}) K^{ijk}_{\alpha\gamma}
\]

The index calculus is fully developed by Kirby and Logg in *A Compiler for Variational Forms.*
Isoparametric Jacobians also give rise to multilinear forms

\[
\int_{\mathcal{T}} \nabla \phi_i(x) \cdot \nabla \phi_j(x) dA \quad (14)
\]

\[
= \int_{\mathcal{T}} \frac{\partial \phi_i(x)}{\partial x_\alpha} \frac{\partial \phi_j(x)}{\partial x_\alpha} dA \quad (15)
\]

\[
= \int_{\mathcal{T}_{\text{ref}}} \frac{\partial \xi_\beta}{\partial x_\alpha} \frac{\partial \phi_i(\xi)}{\partial \xi_\gamma} \frac{\partial \phi_j(\xi)}{\partial \xi_\gamma} |J| dA \quad (16)
\]

\[
= |J| \int_{\mathcal{T}_{\text{ref}}} \phi_k J_k^{\beta \alpha} \frac{\partial \phi_i(\xi)}{\partial \xi_\beta} \phi_l J_l^{\gamma \alpha} \frac{\partial \phi_j(\xi)}{\partial \xi_\gamma} dA \quad (17)
\]

\[
= J_k^{\beta \alpha} J_l^{\gamma \alpha} |J| \int_{\mathcal{T}_{\text{ref}}} \phi_k \frac{\partial \phi_i(\xi)}{\partial \xi_\beta} \phi_l \frac{\partial \phi_j(\xi)}{\partial \xi_\gamma} dA \quad (18)
\]

\[
= G_{\beta \gamma}^{\beta \gamma} (T) K_{ijkl}^{ijkl} \quad (19)
\]

A different space could also be used for Jacobians
from ffc.analysis import analyze_forms
from ffc.compiler import compute_ir

parameters = ffc.default_parameters()
parameters["representation"] = "tensor"
analysis = analyze_forms([a,L], {}, parameters)
ir = compute_ir(analysis, parameters)

a_K = ir[2][0]["AK"][0][0]
a_G = ir[2][0]["AK"][0][1]

K = a_K.A0.astype(numpy.float32)
G = a_G
We generate different computations on the fly,
and can change

- Element Batch Size
- Number of Concurrent Elements
- Loop unrolling
- Interleaving stores with computation
Figure: Tensor Contraction $G^\beta\gamma(T)K^{ij}_{\beta\gamma}$
Figure: Tensor Contraction $G^{\beta\gamma}(\mathcal{T})K^{ij}_{\beta\gamma}$
Computational Flexibility

Basic Contraction

Figure: Tensor Contraction $G^{\beta\gamma}(T)K_{\beta\gamma}^{ij}$
Figure: Tensor Contraction $G^{\beta\gamma}(T)K^{ij}_{\beta\gamma}$
Computational Flexibility
Element Batch Size

Figure: Tensor Contraction $G^{\beta\gamma}(T)K_{\beta\gamma}^{ij}$
Figure: Tensor Contraction $G^{\beta\gamma}(T)K^{ii}_{\beta\gamma}$
Computational Flexibility
Element Batch Size

Figure: Tensor Contraction $G^{\beta\gamma}(T)K^{ij}_{\beta\gamma}$
**Computational Flexibility**

Element Batch Size

![Diagram showing tensor contraction](image)

**Figure:** Tensor Contraction $G^{\beta\gamma}(T)K^{ii\beta\gamma}$
Figure: Tensor Contraction

\[ \beta \gamma \left( T \right) K_{ij}^{\beta \gamma} \]
Computational Flexibility
Concurrent Elements

Figure: Tensor Contraction

\[ K_{\beta\gamma} \]
Computational Flexibility

Concurrent Elements

Figure: Tensor Contraction

$K_{\beta\gamma} (T)_{ij \beta\gamma}$
Computational Flexibility
Concurrent Elements

Figure: Tensor Contraction

\[ \beta \gamma (T) K_{ij} \beta \gamma \]

thread 0
thread 5
thread 15
thread 16
thread 21
thread 31
/* G K contraction: unroll = full */
E[0] += G[0] * K[0];
E[0] += G[1] * K[1];
E[0] += G[7] * K[7];
E[0] += G[8] * K[8];
/ * G K contraction: unroll = none */
for(int b = 0; b < 1; ++b) {
    const int n = b*1;
    for(int alpha = 0; alpha < 3; ++alpha) {
        for(int beta = 0; beta < 3; ++beta) {
            E[b] += G[n*9+alpha*3+beta] * K[alpha*3+beta];
        }
    }
}
/* G K contraction: unroll = none */
for (int b = 0; b < 4; ++b) {
    const int n = b*1;
    for (int alpha = 0; alpha < 3; ++alpha) {
        for (int beta = 0; beta < 3; ++beta) {
            E[b] += G[n*9+alpha*3+beta] * K[alpha*3+beta];
        }
    }
}

/* Store contraction results */
elemMat[Eoffset+idx+0] = E[0];
elemMat[Eoffset+idx+16] = E[1];
elemMat[Eoffset+idx+32] = E[2];
elemMat[Eoffset+idx+48] = E[3];
n = 0;
for (int alpha = 0; alpha < 3; ++alpha) {
    for (int beta = 0; beta < 3; ++beta) {
        E += G[n*9+alpha*3+beta] * K[alpha*3+beta];
    }
}

/* Store contraction result */
elemMat[Eoffset+idx+0] = E;
n = 1; E = 0.0; /* contract */
elemMat[Eoffset+idx+16] = E;
n = 2; E = 0.0; /* contract */
elemMat[Eoffset+idx+32] = E;
n = 3; E = 0.0; /* contract */
elemMat[Eoffset+idx+48] = E;
FEM-GPU

- Analytic Flexibility
- Computational Flexibility
- Efficiency
Performance

Peak Performance

GPU Flop Rate for
3D $P_1$ Lagrange Laplacian and 2D $P_1$ Lagrange Elasticity

- Blue line: Laplacian bs128 ce2 is
- Green line: Elasticity bs256 ce2 is

MFlops/s vs Number of Elements
Price-Performance Comparison of CPU and GPU
3D $P_1$ Laplacian Integration

<table>
<thead>
<tr>
<th>Model</th>
<th>Price ($)</th>
<th>GF/s</th>
<th>MF/s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>GTX285</td>
<td>390</td>
<td>90</td>
<td>231</td>
</tr>
<tr>
<td>Core 2 Duo</td>
<td>300</td>
<td>2</td>
<td>6.6</td>
</tr>
</tbody>
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Price-Performance Comparison of CPU and GPU
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</tr>
<tr>
<td>Core 2 Duo</td>
<td>300</td>
<td>12*</td>
<td>40</td>
</tr>
</tbody>
</table>

* Jed Brown Optimization Engine
Performance
Influence of Element Batch Sizes

CPU vs. GPU Flop Rate for 2D $P_1$ Lagrange ['Elasticity']

Interleave Stores = 1
Loop Unrolling = full

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PDE on GPU
IMA '10
Explaining performance

- Increase shared memory and work/thread until you top out
  - Occupancies go down or level out as performance goes up

- Does not work without interleaved stores
  - Scheduler can switch to kernels who are computing
  - Larger number of smaller computations makes better fit

- Should I worry about detailed explanations for performance?
  - Sensible decompositions, coupled with exploration
  - FLAME methodology
Automated Tuning System

Components of our performance evaluation system:

- Generate set of kernels using:
  - Loop slicing, store reordering, etc.
  - Loop invariants ala FLAME
  - High level constructs ala Rheagen and FEniCS

- Store results and metadata in HDF5 using PyTables
  - Thousands of tests for this talk

- Interrogate and plot with Matplotlib

- Eventually couple to build system
  - FFTW, Spiral, FLAME
Structured code generation, can allow easy integration of novel hardware and reconcile user physics with system traversals.
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2. FEM-GPU
3. FMM-GPU
   • Quick FMM Intro
   • Differences on the GPU
Outline

3 FMM-GPU
  • Quick FMM Intro
  • Differences on the GPU
FMM Applications

FMM can accelerate both integral and boundary element methods for:

- Laplace
- Stokes
- Elasticity
FMM Applications

FMM can accelerate both integral and boundary element methods for:
- Laplace
- Stokes
- Elasticity

Advantages
- Mesh-free
- $O(N)$ time
- Distributed and multicore (GPU) parallelism
- Small memory bandwidth requirement
FMM accelerates the calculation of the function:

\[ \Phi(x_i) = \sum_j K(x_i, x_j)q(x_j) \]  

(20)

- Accelerates \( \mathcal{O}(N^2) \) to \( \mathcal{O}(N) \) time
- The kernel \( K(x_i, x_j) \) must decay quickly from \( (x_i, x_i) \)
  - Can be singular on the diagonal (Calderón-Zygmund operator)
- Discovered by Leslie Greengard and Vladimir Rohklin in 1987
- Very similar to recent wavelet techniques
FMM accelerates the calculation of the function:

\[ \Phi(x_i) = \sum_j \frac{q_j}{|x_i - x_j|} \]  \hspace{1cm} (20)

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PetFMM is an freely available implementation of the Fast Multipole Method
http://barbagroup.bu.edu/Barba_group/PetFMM.html

- Leverages PETSc
  - Same open source license
  - Uses Sieve for parallelism
- Extensible design in C++
  - Templated over the kernel
  - Templated over traversal for evaluation
- MPI implementation
  - Novel parallel strategy for anisotropic/sparse particle distributions
  - PetFMM–A dynamically load-balancing parallel fast multipole library
  - 86% efficient strong scaling on 64 procs
- Example application using the Vortex Method for fluids
- (coming soon) GPU implementation
Spatial Decomposition

Pairs of boxes are divided into *near* and *far*:
Pairs of boxes are divided into *near* and *far*:

Neighbors are treated as *very near*. 
Functional Decomposition

Upward Sweep

Create Multipole Expansions.

P2M  M2M

Evaluate Local Expansions.

M2L  L2L  L2P
Outline

3 FMM-GPU
- Quick FMM Intro
- Differences on the GPU
Multipole-to-Local Transformation

Re-expands a multipole series as a Taylor series

- Up to 85% of time in FMM
  - Tradeoff with direct interaction
- Dense matrix multiplication
  - $2p^2$ rows
- Each interaction list box
  - $(6^d - 3^d) 2^{dL}$
- $d = 2, L = 8$
  - 1,769,472 matvecs
One thread per M2L transform

- Thread block (TB) transforms one Multipole Expansion (ME) for each Interaction List (IL) box — 27 times
  - $p = 12$
  - Matrix size is 2304 bytes
  - Plenty of work per thread (81 Kflops or 36 flops/byte)
  - **BUT**, 16K shared memory only holds 7 matrices
One thread per M2L transform

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GPU M2L
Version 0

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Memory limits concurrency!
Apply M2L transform matrix-free

\[ m_{2l_{ij}} = -1^i \binom{i+j}{j} t^{i-j-1} \]  

- Traverse matrix by perdiagonals
  - Same work
  - No memory limit on concurrency
  - 8 concurrent TBs per MultiProcessor (MP)
  - \(27 \times 8 = 216\) threads, **BUT** max is 512
Apply M2L transform matrix-free

\[ m2l_{ij} = -1^i \binom{i+j}{j} t^{-i-j-1} \]  

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- \( 27 \times 8 = 216 \) threads, **BUT** max is 512

20 GFlops

5x Speedup of Downward Sweep
Apply M2L transform matrix-free

\[ m_{2l_{ij}} = -1^i \binom{i+j}{j} t^{-i-j-1} \]  

- Traverse matrix by perdiagonals
- Same work
- No memory limit on concurrency
- 8 concurrent TBs per MultiProcessor (MP)
- \( 27 \times 8 = 216 \) threads, **BUT** max is 512

20 GFlops

5x Speedup of Downward Sweep

Algorithm limits concurrency!
Apply M2L transform matrix-free

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(21)

Additional problems: Not enough parallelism for data movement
- Move 27 LE to global memory per TB
- \(27 \times 2p = 648\) floats
- With 32 threads, takes 21 memory transactions
One thread per *element* of the LE

\[
m2l_{ij} = -1^i \binom{i + j}{j} t^{-i-j-1}
\]  

- Each thread does a dot product
- Cannot use diagonal traversal, more work
- Avoid branching
  - Each row precomputes \( t^{-i-1} \)
  - All threads loop to \( p + 1 \), only store \( t^{-i-1} \)
- Loop unrolling
- No thread synchronization
One thread per element of the LE

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GPU M2L
Version 2

One thread per *element* of the LE

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300 GFlops

15x Speedup of Downward Sweep
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300 GFlops
15x Speedup of Downward Sweep

Examine memory access
Superior GPU memory bandwidth is due to both

*bus width* and *clock speed*.

<table>
<thead>
<tr>
<th></th>
<th>CPU</th>
<th>GPU</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bus Width (bits)</td>
<td>64</td>
<td>512</td>
</tr>
<tr>
<td>Bus Clock Speed (MHz)</td>
<td>400</td>
<td>1600</td>
</tr>
<tr>
<td>Memory Bandwidth (GB/s)</td>
<td>3</td>
<td>102</td>
</tr>
<tr>
<td>Latency (cycles)</td>
<td>240</td>
<td>600</td>
</tr>
</tbody>
</table>

Tesla always accesses blocks of 64 or 128 bytes.
Coalesce and overlap memory accesses

Coalescing is

- a group of 16 threads
- accessing consecutive addresses
  - 4, 8, or 16 bytes
- in the same block of memory
  - 32, 64, or 128 bytes
Coalesce and overlap memory accesses
Memory accesses can be overlapped with computation when

- a TB is waiting for data from main memory
- another TB can be scheduled on the SM
- 512 TB can be active at once on Tesla
Coalesce and overlap memory accesses

Note that the theoretical peak (1 TF)
- MULT and FMA must execute simultaneously
- 346 GOps
- Without this, peak can be closer to 600 GF

480 GFlops
25x Speedup of Downward Sweep
Design Principles

M2L required all of these optimization steps:

- Many threads per kernel
- Avoid branching
- Unroll loops
- Coalesce memory accesses
- Overlap main memory access with computation
How Will Algorithms Change?

Massive concurrency is necessary
- Mix of vector and thread paradigms
- Demands new analysis

More attention to memory management
- Blocks will only get larger
- Determinant of performance