Advanced Topics in Numerical Analysis: High Performance Computing

Intro to GPGPU

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Spring 2019, Monday, 5:10–7:00PM, WWH #1302

April 8, 2019

Outline

Organization

Scheduling:

- Homework assignment #4 due next Monday

Topics today:

- Final project overview/discussion
- More GPGPU programming (several examples)
- Algorithms: image filtering (convolution), parallel scan, bitonic sort

Outlook for next week(s):

- Distributed memory programming (MPI)

Outline

Organization issues

Final projects

Computing on GPUs

Final projects

- Final projects! Pitch/discuss your final project to/with us. We're available Tuesday (tomorrow) 5-6pm and Thursday 11-12:30 in WWH #1111 or over Slack.
- Would like to (more or less) finalize project groups and topics in the next week.
- Final projects are in teams of 1-3 people (2 preferred!)
- We posted suggestions for final projects. More ideas on the next slides. Also, take a look at the HPC projects we collected from the first homework assignment.
- Final project presentations (max 10min each) in the week May 20/21. You are also required to hand in a short paper with your results, as well as the git repo with the code.

Final projects

Final project examples (from example list):

- Parallel multigrid
- Image denoising
- Adaptive finite volumes
- Parallel k-means
- Fluid mechanics simulation
- Data partitioning using parallel octrees

Final projects

Final project examples (more examples):

- Parallelizing a DFT sub-calculation (Tkatchenko-Scheffler dispersion energies and forces)
- Parallelizing a neural network color transfer method for images
- Parallel all-pairs shortest paths via Floyd-Warshall
- Fast CUDA kernels for ResNet inference
- ... Take an existing serious code and speed it up/parallelize it
- ...

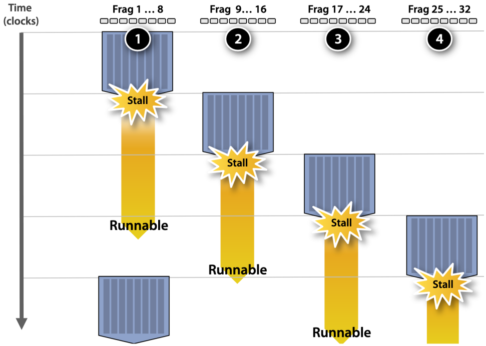
Outline

Review of Last Class

- **CUDA programming model:** GPU architecture, memory-hierarchy, thread-hierarchy.
- **Shared memory:** fast, low-latency, shared within thread-block, 48KB - 128KB (depending on compute capability)
  - avoid bank conflicts within a warp.
- **Synchronization**
  - **__syncthreads()** all threads in a block
  - **__syncwarp()** all threads in a warp
- **Reduction on GPUs**

Hiding Latency

- All operations have latency
- CPUs hide latency using out-of-order computation and branch prediction; reduce latency of memory accesses using caches.
- GPUs hide latency using parallelism:
  - execute warp-1 (threads 0-31)
  - when warp-1 stalls, start executing warp-2 (threads 32-63) and so on $\cdots$



Credit: Kayvon Fatahalian (Stanford)

Occupancy Calculator

Get resource usage for kernel functions (compiler flag: **-Xptxas -v**)

Example:

```
# nvcc -std=c++11 -Xcompiler "-fopenmp" -Xptxas -v reduction.cu

ptxas info :  Compiling entry function
'_Z16reduction_kernelPdPKdl' for 'sm_30'
ptxas info :  Function properties for _Z16reduction_kernelPdPKdl
0 bytes stack frame, 0 bytes spill stores, 0 bytes spill loads
ptxas info :  Used 28 registers, 8192 bytes smem, 344 bytes cmem[0]
```

$$\text{Occupancy} = \frac{\#\text{-of-threads per SM}}{\text{max-}\#\text{-of-threads per SM}}$$

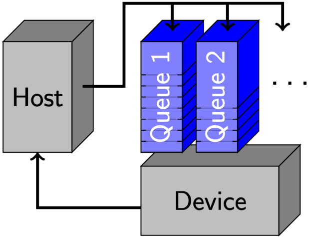
- Calculate occupancy for your code:
  - https://developer.download.nvidia.com/compute/cuda/CUDA_Occupancy_calculator.xls
  - web version: https://xmartlabs.github.io/cuda-calculator
  - **Improve occupancy to improve performance**

Device Management (Multiple GPUs)

- Get number of GPUs: **cudaGetDeviceCount(int *count)**
- Set the current GPU: **cudaSetDevice(int device)**
- Get current GPU: **cudaGetDevice(int *device)**
- Get GPU properties: **cudaGetDeviceProperties(cudaDeviceProp *prop, int device)**

Streams

- execute multiple tasks in parallel; either on separate GPUs or on the same GPU.
- useful for executing several independent small tasks where each task does not have sufficient parallelism.




```
// create streams
cudaStream_t stream1, stream2
cudaStreamCreate(&streams1);
cudaStreamCreate(&streams2);

// launch two kernels in parallel
kernel<<<1, 64, 0, streams1>>>();
kernel<<<1, 128, 0, streams2>>>();

// synchronize
cudaStreamSynchronize(stream1)
cudaStreamSynchronize(stream2)
```

Image Filtering

Convolution: read $k \times k$ block of the image multiply by filter weights and sum.

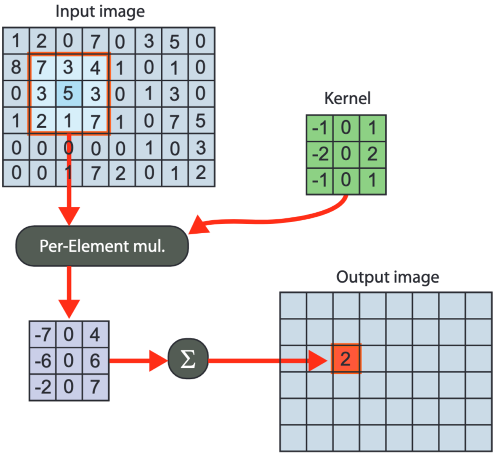


figure from: GPU Computing: Image Convolution - Jan Novák, Gábor Liktor, Carsten Dachsbacher

Image Filtering

Using shared memory as cache to minimize global memory reads

- read a 32×32 block of original image from main memory
- compute convolution in shared memory
- write back result sub-block (excluding halo)

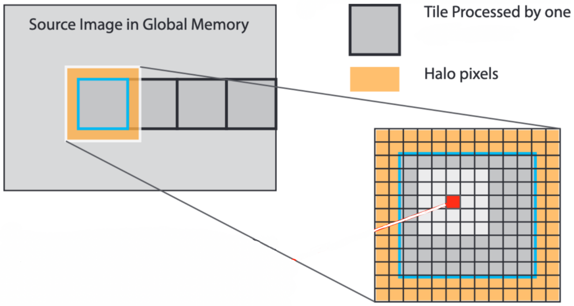


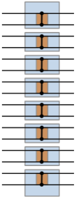
figure from: GPU Computing: Image Convolution - Jan Novák, Gábor Liktor, Carsten Dachsbacher

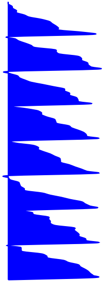
Sorting

Comparison based sorting algorithms: bubble sort $\mathcal{O}(N^2)$, sample sort $\mathcal{O}(N \log N)$, merge sort $\mathcal{O}(N \log N)$

Bitonic merge sort $\mathcal{O}(N \log^2 N)$

- great for small to medium problem sizes.
- sorting networks, simple deterministic algorithm bases on compare and swap.
- sequence of $\log N$ **bitonic merge** operations.





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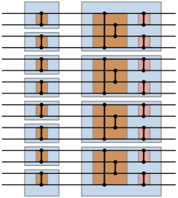

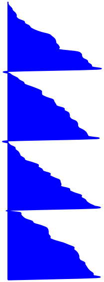

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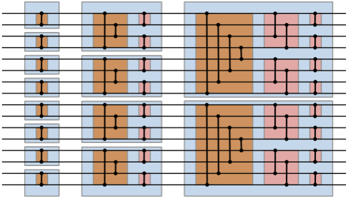

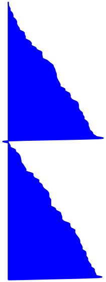

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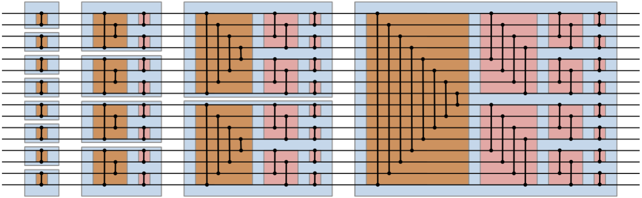
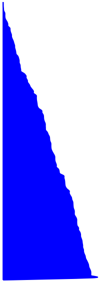
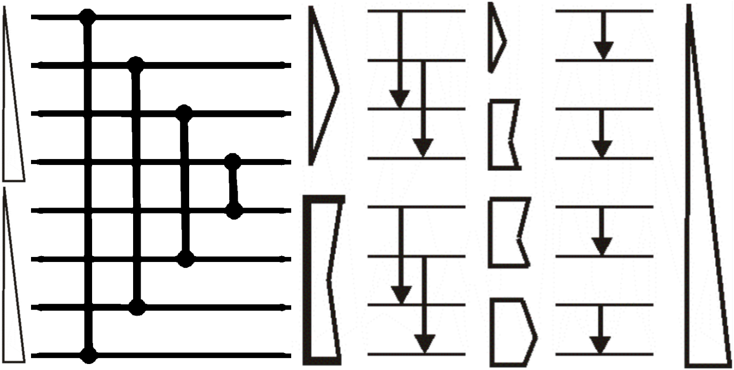




Bitonic Sort

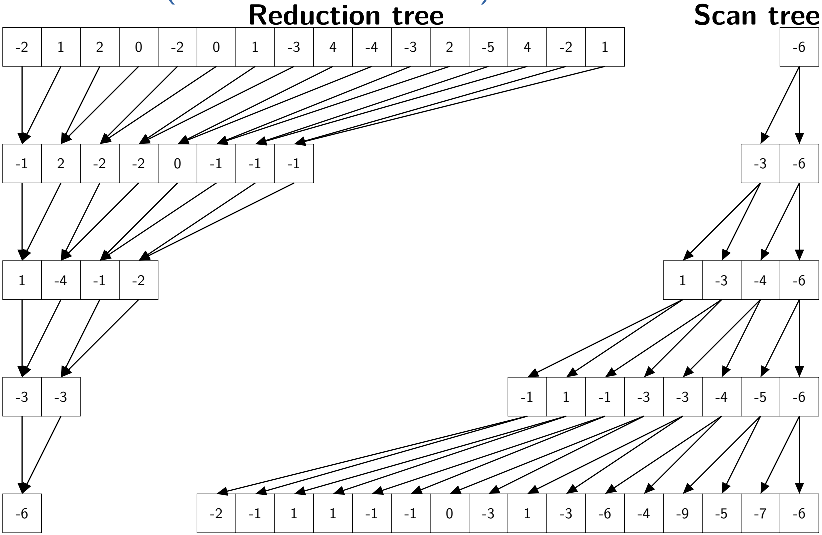
Bitonic merge $\mathcal{O}(N \log N)$ cost for each merge operation

- divide-and-conquer algorithm on bitonic sequences.
- **Bitonic sequence:** a sequence that changes monotonicity exactly once.



- if bitonic-sequence larger than block-size, then read and write directly from global memory; otherwise read/write from shared-memory

Parallel Scan (within thread-block)



Construct scan tree: right child: copy parent's value.
left child: difference between parent's value and sibling's value in reduction tree.

Libraries

Optimized libraries for

- **cuBLAS** for linear algebra
- **cuFFT** for Fast Fourier Transform
- **cuDNN** for Deep Neural Networks

cuBLAS Demo!

Summary

- **Calculating Occupancy:** higher is better
  - useful for debugging performance bottlenecks
- **Miscellaneous:**
  - managing multiple GPUs
  - executing multiple streams in parallel
- **Algorithms**
  - Image filtering
  - Parallel scan
  - Bitonic sort
- **Libraries:** cuBLAS, cuFFT, cuDNN