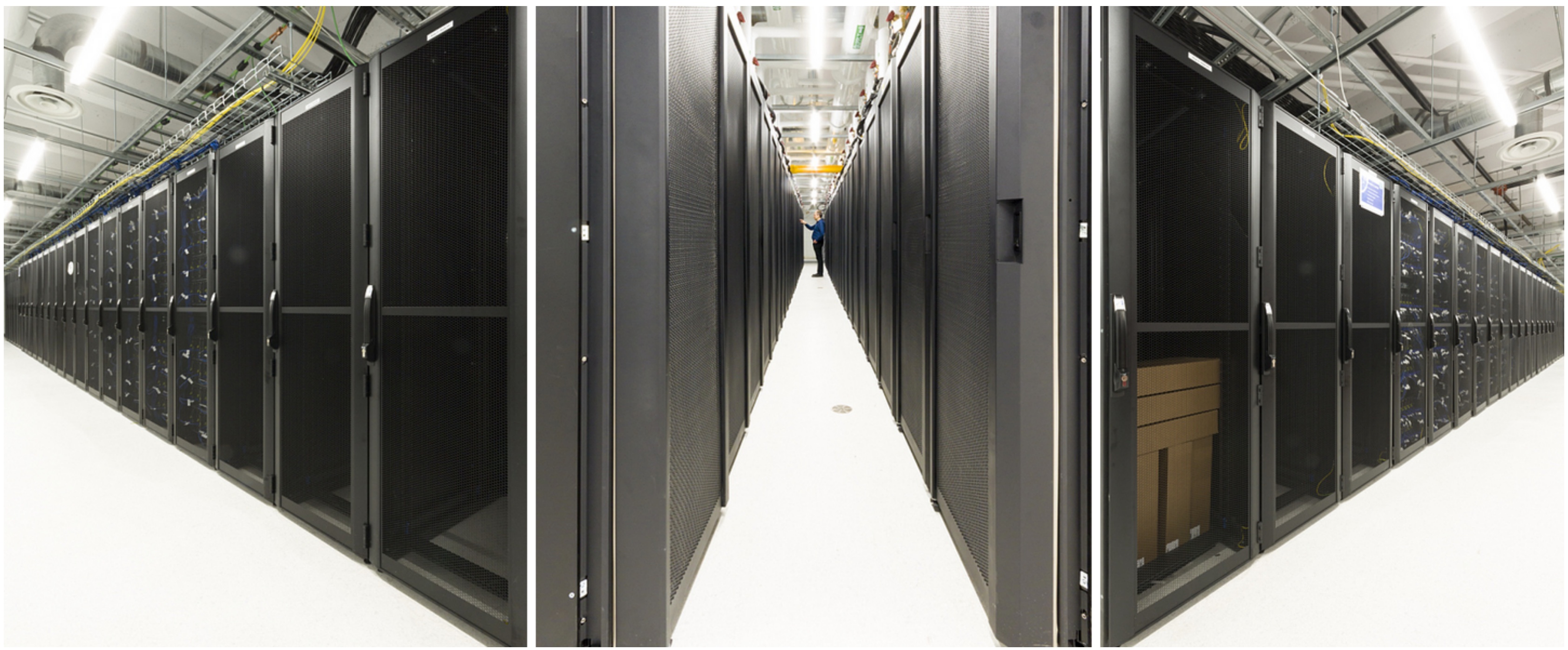
What’s new and exciting about Graham’s GPUs



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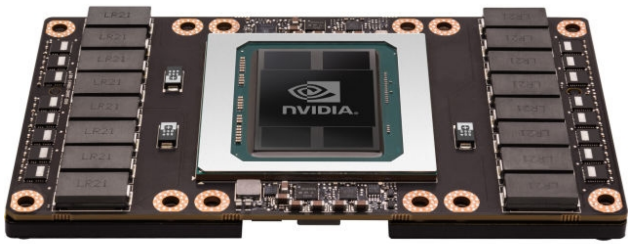
From Fermi to Pascal

- The Monk GPUs are very dated - they are of Fermi generation, and since then NVIDIA introduced Kepler, Maxwell, and Pascal GPU architectures.
  - Fermi: 2010
  - Kepler: 2012
  - [Maxwell: 2014]
  - Pascal: 2016



(Maxwell didn't have any HPC GPUs.)

- The new cluster Graham has 320 of HPC Pascal GPUs, P100. (Cedar at Simon Fraser has 584 P100's.)

Evolutionary changes

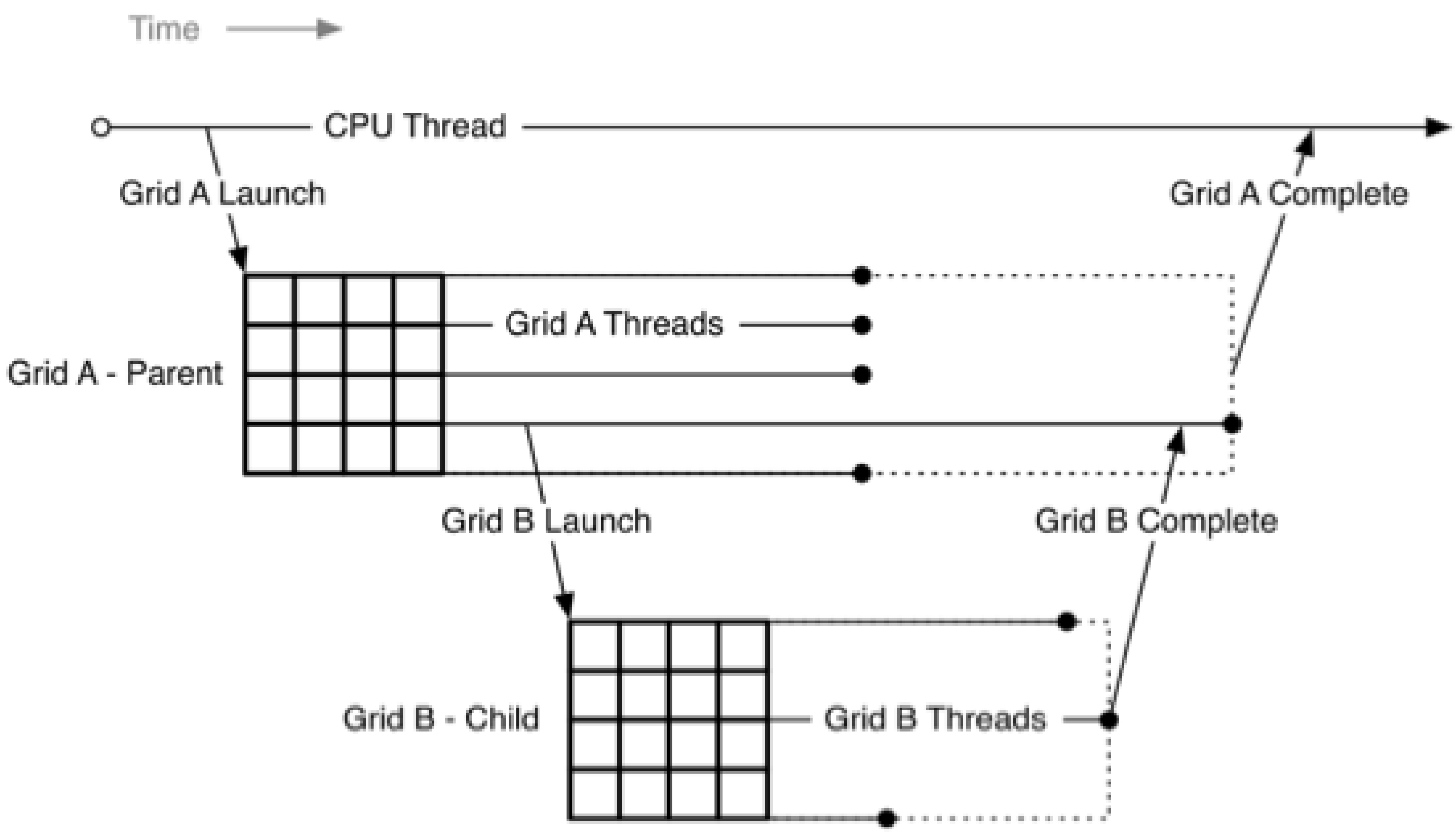
Specification	Monk	Graham
CUDA cores	448	3584
SP flops	1.03 TFlops	9.3 TFlops
Device memory	5.2 GB	12 GB
Memory bandwidth	148 GB/s	549 GB/s

Revolutionary changes

- CUDA Dynamic Parallelism (CDP): new hard/software feature allowing for dynamic workload generation on GPU (kernels launched from kernels). Makes GPU much more general purpose computing device. First appeared in Kepler GPUs.
- Hyper-Q: in previous generations, multiple CPU threads could only access the GPU sequentially (one queue); Kepler / Pascal expand that to 32 parallel queues. This should significantly accelerate mixed MPI/CUDA and OpenMP/CUDA codes, without any code modifications. Also great for GPU farming.

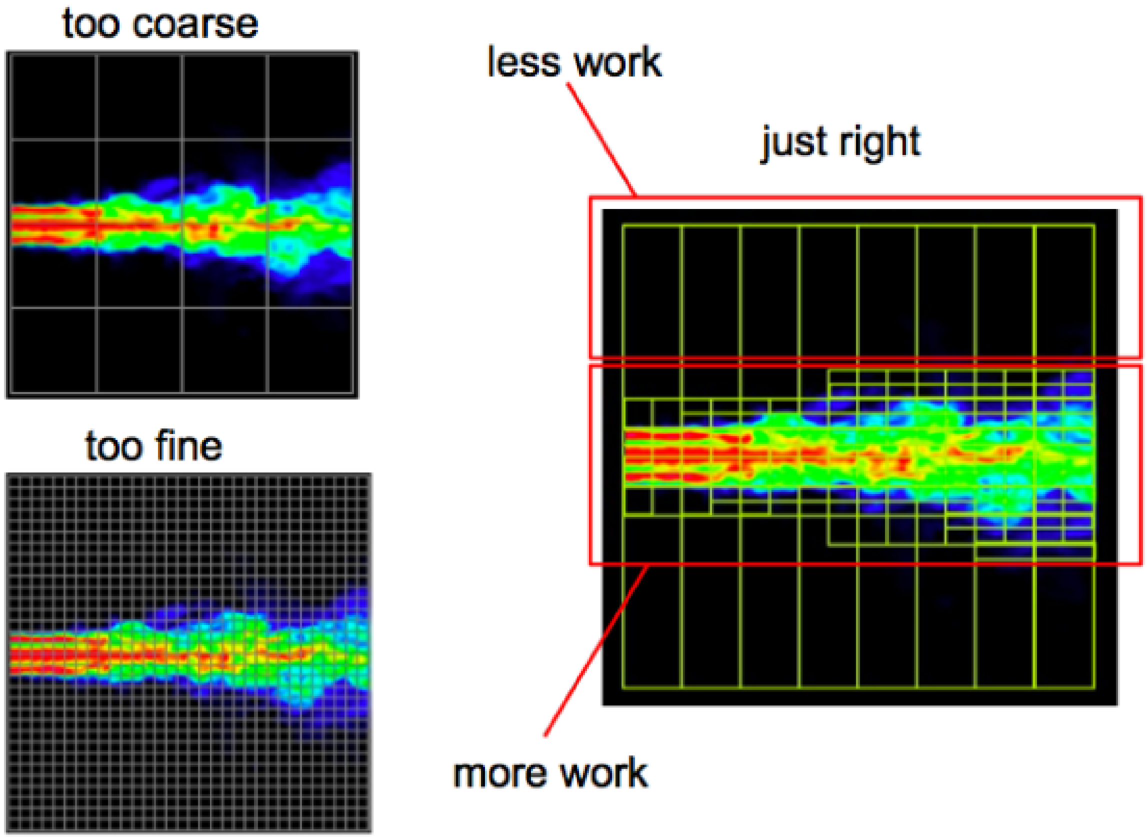
Dynamic Parallelism

- Dynamic parallelism (DP) is available in CUDA 5.0 and later on devices of Compute Capability 3.5 or higher (sm_35 for Kepler; sm_60 for Pascal).
- Under DP, an application can launch a coarse-grained kernel which in turn launches finer-grained kernels to do work where needed.



Dynamic Parallelism

- DP is perfect for adaptive grid codes and codes with recursion.



DP: simple example

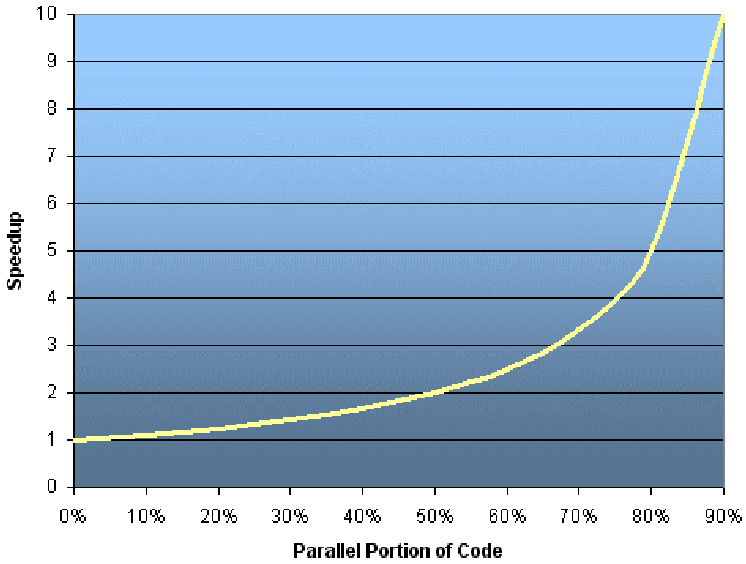
- DP allows one to move almost everything to GPU.

```
// On device:
// Second level kernels (multi-threaded):
__global__  void  kernel1 (){}
__global__  void  kernel2 (){}

// Top level kernel (single-threaded):
__global__ void main_kernel (){
  if (threadIdx.x == 0) {
//  These second level kernels will run sequentially (would need streams for concurrency)
     kernel1<<<Nblocks, Nthreads>>>();
     kernel2<<<Nblocks, Nthreads>>>();
     ...
     }}
// On host:
int main() {
   main_kernel<<<1,1>>>();}
```

Amdahl's Law

- Amdahl's Law states that potential program speedup is defined by the fraction of code (P) that can be parallelized:

$$\textbf{speedup} = \frac{1}{1 - P}$$



- If none of the code can be parallelized, P = 0 and the speedup = 1 (no speedup). If all of the code is parallelized, P = 1 and the speedup is infinite (in theory).
- If 50% of the code can be parallelized, maximum speedup = 2, meaning the code will run twice as fast.

Amdahl's Law (2)

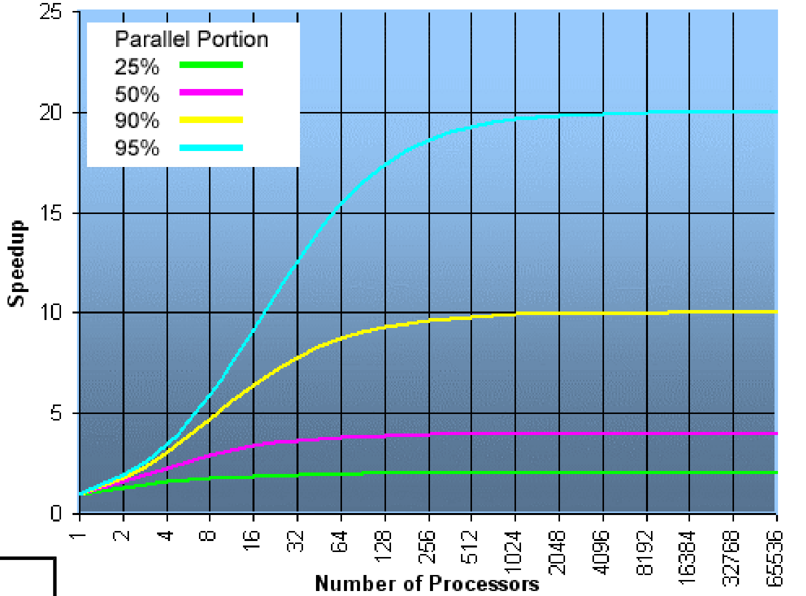
- Introducing the number of processors performing the parallel fraction of work, the relationship can be modeled by:

$$\textbf{speedup} = \frac{1}{\frac{P}{N} + S}$$

where P = parallel fraction, N = number of processors and S = serial fraction.

Amdahl's Law (3)

- It soon becomes obvious that there are limits to the scalability of parallelism. For example, at P = .50, .90 and .99 (50%, 90% and 99% of the code is parallelizable):



	speedup		
N	P = .50	P = .90	P = .99
10	1.82	5.26	9.17
100	1.98	9.17	50.25
1000	1.99	9.91	90.99
10000	1.99	9.91	99.02

Hyper-Q: why is it important?

- GPUs work well when you saturate them with data-parallel threads.
- Graham GPU has 8 times more cores (so need 8x more threads to get saturated) than the Monk GPU.
- From the Amdahl's law, a code which runs well on Monk will likely perform poorly* on Graham.
- Hyper-Q helps to mitigate this, by allowing to share one GPU between different CPU threads.

Live demo of Hyper-Q

- A simple code, primes_HQ, only runs one block of threads per kernel.
- This mimics a realistic code which doesn't have enough of parallelism to saturate a modern GPU.
- Important: Hyper-Q is usually not enabled by default.

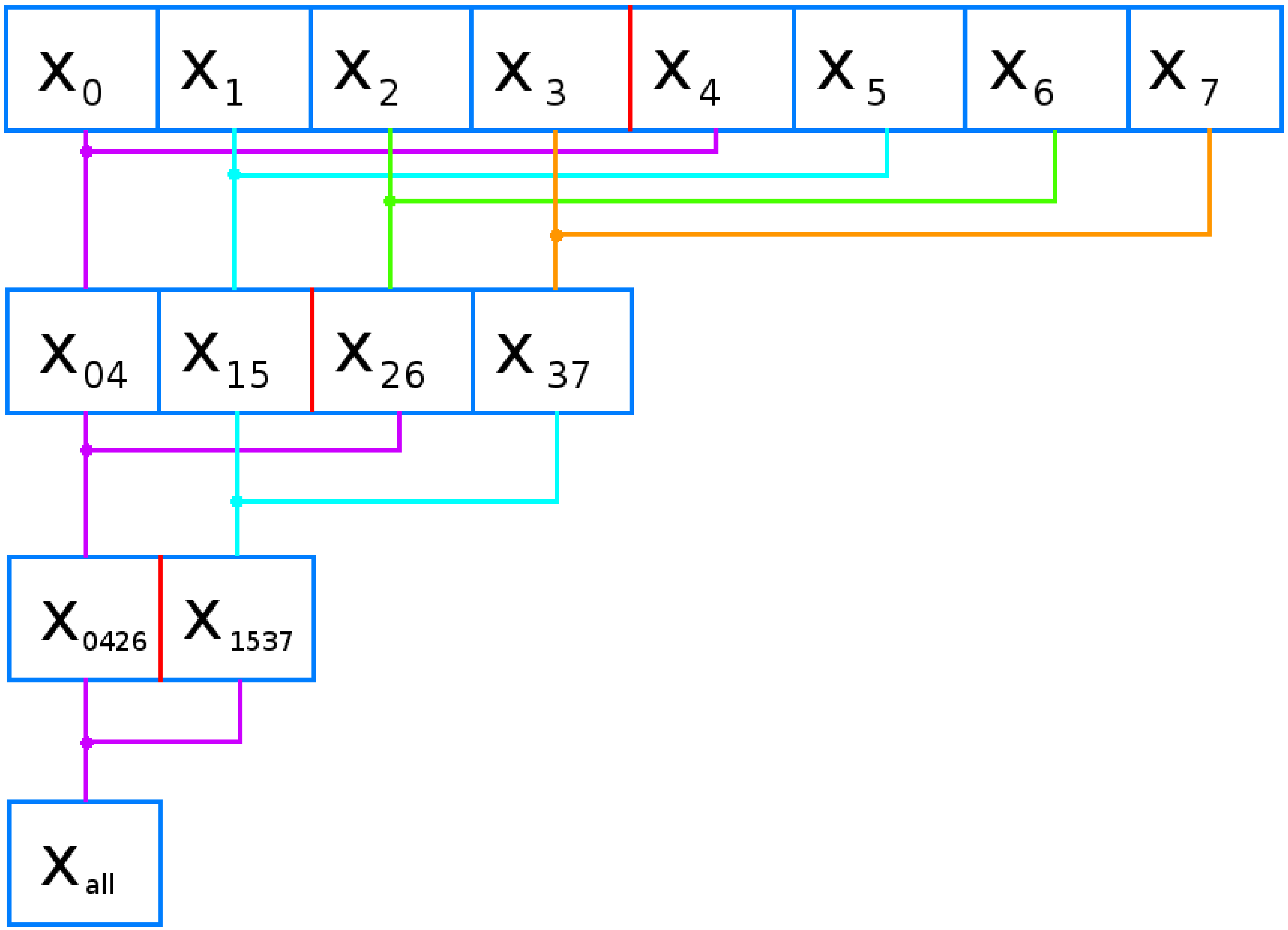
Job script for GPU farming

```
#!/bin/bash
#SBATCH --gres=gpu:1
#SBATCH -t 0-00:30
#SBATCH --mem=4G
#SBATCH -c 16

export CUDA_MPS_LOG_DIRECTORY=$HOME/tmp
nvidia-cuda-mps-control -d

for ((i=0; i<16; i++))
   do
   ./code &>out &
   done
wait
```

Other new features

- Atomic operations improvements:
  - atomicAdd now supports FP64 (integer and float)
  - atomicMin and atomicMax now support INT64
- Half precision (FP16) at twice speed of FP32
- HBM2 memory: much higher bandwidth, hardware ECC (no memory or efficiency wasted for ECC).
- Quantitative improvements:
  - Grid length (1D): 65,535 -> 2e9
  - 32-bit registers per thread: 63 -> 255
  - Concurrent kernels per device: 16 -> 128

Binary reduction



Kernel for binary summation

```
__shared__ double  sum[BLOCK_SIZE];
...
__syncthreads(); // To make sure all sum[] elements were initialized
int nTotalThreads = blockDim.x;  // Total number of active threads;
// only the first half of the threads will be active.


while(nTotalThreads > 1)
{
  int halfPoint = nTotalThreads / 2; // Number of active threads

  if (threadIdx.x < halfPoint)
  {
    int thread2 = threadIdx.x + halfPoint; // the second element index
    sum[threadIdx.x] += sum[thread2];  // Pairwise summation
  }
  __syncthreads();
  nTotalThreads = halfPoint;  // Reducing the binary tree size by two}
```

Binary at the lower level, atomic at the higher level

```
__shared__ float  sum[BLOCK_SIZE];
// Initialize sum[] array here
__syncthreads(); // To make sure all sum[] elements were initialized
int nTotalThreads = blockDim.x;  // Total number of active threads;
// only the first half of the threads will be active.

while(nTotalThreads > 1){
  int halfPoint = nTotalThreads / 2; // Number of active threads

  if (threadIdx.x < halfPoint)
  {
    int thread2 = threadIdx.x + halfPoint; // the second element index
    sum[threadIdx.x] += sum[thread2];  // Pairwise summation
  }
  __syncthreads();
  nTotalThreads = halfPoint;  // Reducing the binary tree size by two
}
if (threadIdx.x == 0)
        atomicAdd (&xsum, sum[0]); // Atomic reduction
```

FP64 reduction on monk

- Two-level binary reduction:

```
// Host code
#define  BSIZE  1024  // Always use a power of two; can be 32...1024
// Total number of elements to process: 1024 < Ntotal < 1024^2

int Nblocks = (Ntotal+BSIZE-1) / BSIZE;

// Low level (the results should be stored in global device memory):
x_prereduce <<<Nblocks, BSIZE >>> ();

// High level (will read the input from global device memory):
x_reduce <<<1, Nblocks >>> ();
```

Online quiz

Link: http://www.socrative.com

Room: CUDADAY2