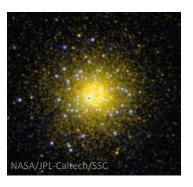
# Parallel Programming

N-Body Simulation in CUDA

Slides based on Martin Burtscher's tutorial

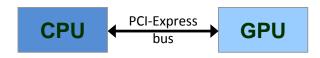
### Outline

- Review: GPU programming
- N-body example
- Porting and tuning



# **CUDA Programming Model**

- Non-graphics programming
  - Uses GPU as massively parallel co-processor



- SIMT (single-instruction multiple-threads) model
  - Thousands of threads needed for full efficiency

- C/C++ with extensions
  - Function launch
    - Calling functions on GPU
  - Memory management
    - GPU memory allocation, copying data to/from GPU
  - Declaration qualifiers
    - Device, shared, local, etc.
  - Special instructions
    - Barriers, fences, etc.
  - Keywords
    - threadIdx, blockIdx

## Calling GPU Kernels

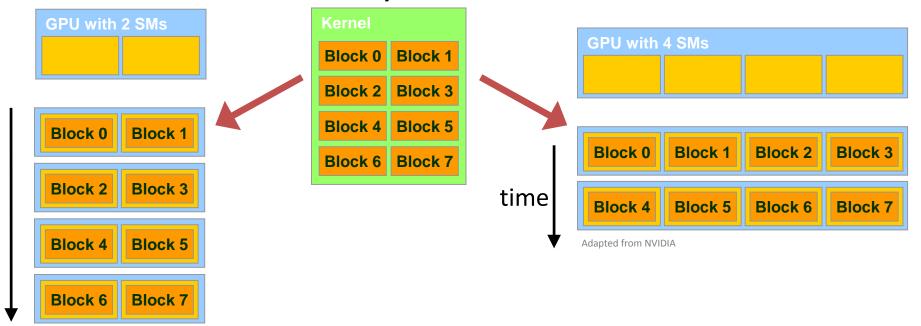
- Kernels are functions that run on the GPU
  - Callable by CPU code
  - CPU can continue processing while GPU runs kernel KernelName<<<m, n>>>(arg1, arg2, ...);
- Launch configuration (programmer selectable)
  - GPU spawns m blocks of n threads per block (i.e., m\*n threads total) that run a copy of the same function
  - Normal function parameters: passed conventionally
    - Different address space

### **GPU Architecture**

 GPUs consist of Streaming Multiprocessors (SMs) - 1 to 30 SMs per chip (run blocks) SMs contain Processing Elements (PEs) - 8, 32, or 192 PEs per SM (run threads) Shared **Global Memory** Adapted from NVIDIA

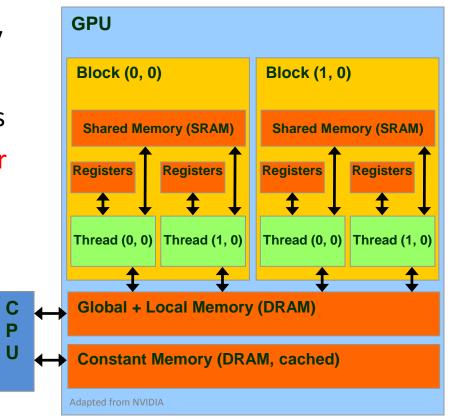
# **Block Scalability**

- Hardware can assign blocks to SMs in any order
  - A kernel with enough blocks scales across GPUs
  - Not all blocks may be resident at the same time



### **GPU Memories**

- Separate from CPU memory
  - CPU can access GPU's global
     & constant mem. via PCIe bus
  - Requires slow explicit transfer
- Visible GPU memory types
  - Registers (per thread)
  - Local mem. (per thread)
  - Shared mem. (per block)
    - Software-controlled cache
  - Global mem. (per kernel)
  - Constant mem. (read only)



Slow communic. between blocks

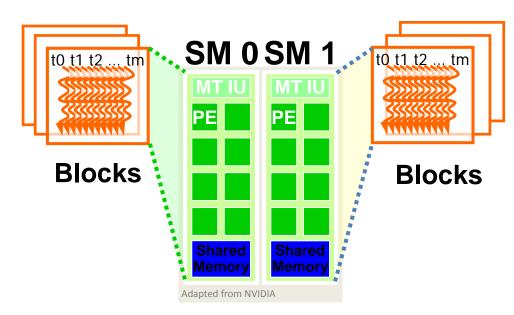
### SM Internals (Fermi and Kepler)

#### Caches

- Software-controlled shared memory
- Hardware-controlled incoherent L1 data cache
- 64 kB combined size, can be split 16/48, 32/32, 48/16
- Synchronization support
  - Fast hardware barrier within block (\_\_syncthreads())
  - Fence instructions: memory consistency & coherency
- Special operations
  - Thread voting (warp-based reduction operations)

### **Block and Thread Allocation Limits**

- Blocks assigned to SMs
  - Until first limit reached
- Threads assigned to PEs



- Hardware limits
  - 8/16 active blocks/SM
  - 1024, 1536, or 2048
     resident threads/SM
  - 512 or 1024 threads/blk
  - 16k, 32k, or 64k regs/SM
  - 16 kB or 48 kB shared memory per SM
  - $-2^{16}-1$  or  $2^{31}-1$  blks/kernel

### Warp-based Execution

- 32 contiguous threads form a warp
  - Execute same instruction in same cycle (or disabled)
  - Warps are scheduled out-of-order with respect to each other to hide latencies
- Thread divergence
  - Some threads in warp jump to different PC than others
  - Hardware runs subsets of warp until they re-converge
  - Results in reduction of parallelism (performance loss)

## Thread Divergence

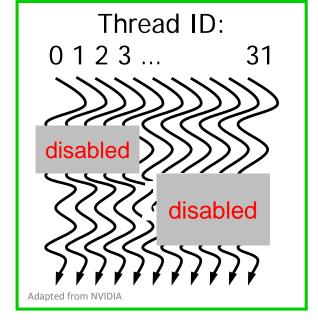
Non-divergent code

```
if (threadID >= 32) {
    some_code;
} else {
    other_code;
}
```



Divergent code

```
if (threadID >= 13) {
    some_code;
} else {
    other_code;
}
```



### Parallel Memory Accesses

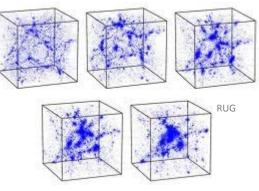
- Coalesced main memory access
  - Under some conditions, HW combines multiple (half) warp memory accesses into a single coalesced access
- Bank-conflict-free shared memory access
  - No superword alignment or contiguity requirements

## Warnings for GPU Programming

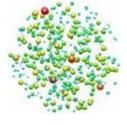
- GPUs can only execute some types of code fast
  - Need lots of data parallelism, data reuse, & regularity
- GPUs are harder to program and tune than CPUs
  - poor tool support
  - architecture
  - poor support for irregular code

## N-body Simulation

- Time evolution of physical system
  - System consists of bodies
  - "n" is the number of bodies
  - Bodies interact via pair-wise forces



- Many systems can be modeled in this way
  - Star/galaxy clusters (gravitational force)
  - Particles (electric force, magnetic force)



### Simple N-body Algorithm

Algorithm

```
Initialize body masses, positions, and velocities
Iterate over time steps {
    Accumulate forces acting on each body
    Update body positions and velocities based on force
}
Output result
```

- More sophisticated n-body algorithms exist
  - Barnes Hut algorithm
  - Fast Multipole Method (FMM)

## Key Loops (Pseudo Code)

```
bodySet = ...; // input
for timestep do { // sequential
  foreach Body b1 in bodySet \{ // O(n^2) \text{ parallel} \}
    foreach Body b2 in bodySet {
      if (b1 != b2) {
        bl.addInteractionForce(b2);
  foreach Body b in bodySet { // O(n) parallel
    b.Advance();
   output result
```

### Force Calculation C Code

```
struct Body {
 float mass, posx, posy, posz; // mass and 3D position
 float velx, vely, velz, accx, accy, accz; // 3D velocity & accel
} *body;
for (i = 0; i < nbodies; i++) {
 for (j = 0; j < nbodies; j++) {
    if (i != j) {
     dx = body[j].posx - px; // delta x
     dy = body[j].posy - py; // delta y
     dz = body[j].posz - pz; // delta z
     dsq = dx*dx + dy*dy + dz*dz; // distance squared
     dinv = 1.0f / sqrtf(dsq + epssq); // inverse distance
      scale = body[j].mass * dinv * dinv * dinv; // scaled force
     ax += dx * scale; // accumulate x contribution of accel
      ay += dy * scale; az += dz * scale; // ditto for y and z
```

### N-body Algorithm Suitability for GPU

- Lots of data parallelism
  - Force calculations are independent
  - Should be able to keep SMs and PEs busy
- Sufficient memory access regularity
  - All force calculations access body data in same order
  - Should have lots of coalesced memory accesses
- Sufficient code regularity
  - All force calculations are identical
  - There should be little thread divergence
- Plenty of data reuse
  - $O(n^2)$  operations on O(n) data
  - CPU/GPU transfer time is insignificant

### C to CUDA Conversion

- Two CUDA kernels
  - Force calculation
  - Advance position and velocity
- Benefits
  - Force calculation requires over 99.9% of runtime
    - Primary target for acceleration
  - Advancing kernel unimportant to runtime
    - But allows to keep data on GPU during entire simulation
    - Minimizes GPU/CPU transfers

### C to CUDA Conversion

```
global void ForceCalcKernel(int nbodies, struct Body *body, ...) {
 global void AdvancingKernel(int nbodies, struct Body *body, ...) {
int main(...) {
 Body *body, *bodyl;
 cudaMalloc((void**)&bodyl, sizeof(Body)*nbodies);
 cudaMemcpy(bodyl, body, sizeof(Body)*nbodies, cuda...HostToDevice);
 for (timestep = ...) {
   ForceCalcKernel<<<1, 1>>>(nbodies, bodyl, ...);
   AdvancingKernel <<<1, 1>>> (nbodies, bodyl, ...);
  cudaMemcpy(body, bodyl, sizeof(Body)*nbodies, cuda...DeviceToHost);
 cudaFree(bodyl);
```

### **Evaluation Methodology**

- Systems and compilers
  - CC 1.3: Quadro FX 5800, nvcc 3.2
    - 30 SMs, 240 PEs, 1.3 GHz, 30720 resident threads
  - CC 2.0: Tesla C2050, nvcc 3.2
    - 14 SMs, 448 PEs, 1.15 GHz, 21504 resident threads
  - CC 3.0: GeForce GTX 680, nvcc 4.2
    - 8 SMs, 1536 PEs, 1.0 GHz, 16384 resident threads
- Input and metric
  - 1k, 10k, or 100k star clusters (Plummer model)
  - Median runtime of three experiments, excluding I/O

### 1-Thread Performance

#### Problem size

- n=10000, step=1
- n=10000, step=1
- n=3000, step=1

### Slowdown rel. to CPU

- CC 1.3: 72.4
- CC 2.0: 36.7
- CC 3.0: 68.1

(Note: comparing different GPUs to different CPUs)

#### Performance

 1 thread is one to two orders of magnitude slower on GPU than CPU

#### Reasons

- No caches (CC 1.3)
- Not superscalar
- Slower clock frequency
- No SMT latency hiding

## Using N Threads

- Approach
  - Eliminate outer loop
  - Instantiate n copies of inner loop, one per body
- Threading
  - Blocks can only hold 512 or 1024 threads
    - Up to 8/16 blocks can be resident in an SM at a time
    - SM can hold 1024, 1536, or 2048 threads
    - Use 256 threads per block (works for all three GPUs)
  - Need multiple blocks
    - Last block may not need all of its threads

# Using N Threads

```
global void ForceCalcKernel(int nbodies, struct Body *body, ...) {
 for (i = 0; i < nbodies; i++) {</pre>
 i = threadIdx.x + blockIdx.x * blockDim.x; // compute i
  if (i < nbodies) { // in case last block is only partially used</pre>
    for (j = ...) {
 global void AdvancingKernel(int nbodies,...) // same changes
#define threads 256
int main(...) {
  int blocks = (nbodies + threads - 1) / threads; // compute block cnt
 for (timestep = ...) {
   ForceCalcKernel<<<1, 1blocks, threads>>>(nbodies, bodyl, ...);
   AdvancingKernel<<<1, 1blocks, threads>>>(nbodies, bodyl, ...);
```

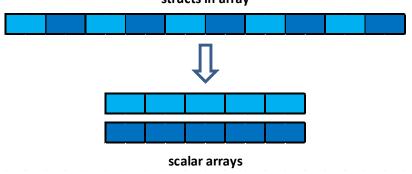
## N Thread Speedup

- Relative to 1 GPU thread
  - CC 1.3: 7781 (240 PEs)
  - CC 2.0: 6495 (448 PEs)
  - CC 3.0: 12150 (1536 PEs)
- Relative to 1 CPU thread
  - CC 1.3: 107.5
  - CC 2.0: 176.7
  - CC 3.0: 176.2

- Performance
  - Speedup much higher
     than number of PEs
     (32, 14.5, and 7.9 times)
  - Due to SMT latency hiding
- Per-core performance
  - CPU core delivers up to
     4.4, 5, and 8.7 times as
     much performance as a
     GPU core (PE)

### **Using Scalar Arrays**

- Data structure conversion
  - Arrays of structs are bad for coalescing
  - Bodies' elements (e.g., mass fields) are not adjacent
- Optimize data structure
  - Use multiple scalar arrays, one per field (need 10)
  - Results in code bloat but often much better speed



# **Using Scalar Arrays**

```
_global__ void ForceCalcKernel(int nbodies, float *mass, ...) {
 // change all "body[k].blah" to "blah[k]"
 global void AdvancingKernel(int nbodies, float *mass, ...) {
 // change all "body[k].blah" to "blah[k]"
int main(...) {
 float *mass, *posx, *posy, *posz, *velx, *vely, *velz, *accx, *accy, *accz;
  float *massl, *posxl, *posyl, *poszl, *velxl, *velyl, *velzl, ...;
 mass = (float *)malloc(sizeof(float) * nbodies); // etc
  cudaMalloc((void**)&massl, sizeof(float)*nbodies); // etc
  cudaMemcpy(massl, mass, sizeof(float)*nbodies, cuda...HostToDevice); // etc
  for (timestep = ...) {
   ForceCalcKernel<<<blooks, threads>>>(nbodies, massl, posxl, ...);
   AdvancingKernel << blocks, threads>>> (nbodies, massl, posxl, ...);
  cudaMemcpy(mass, massl, sizeof(float)*nbodies, cuda...DeviceToHost); // etc
```

## Scalar Array Speedup

- Problem size
  - n=100000, step=1
  - n=100000, step=1
  - n=300000, step=1
- Relative to struct
  - CC 1.3: 0.83
  - CC 2.0: 0.96
  - CC 3.0: 0.82

- Performance
  - Threads access same memory locations, not adjacent ones
    - Always combined but not really coalesced access
  - Slowdowns may be due to DRAM page/TLB misses
- Scalar arrays
  - Still needed (see later)

### **Constant Kernel Parameters**

- Kernel parameters
  - Lots of parameters due to scalar arrays
  - All but one parameter never change their value
- Constant memory
  - "Pass" parameters only once
  - Copy them into GPU's constant memory
- Performance implications
  - Reduced parameter passing overhead
  - Constant memory has hardware cache

### **Constant Kernel Parameters**

```
constant int nbodiesd:
 constant float dthfd, epssqd, float *massd, *posxd, ...;
 global void ForceCalcKernel(int step) {
 // rename affected variables (add "d" to name)
__global__ void AdvancingKernel() {
 // rename affected variables (add "d" to name)
int main(...) {
  cudaMemcpyToSymbol(massd, &massl, sizeof(void *)); // etc
  for (timestep = ...) {
   ForceCalcKernel<<<1, 1>>>(step);
   AdvancingKernel<<<1, 1>>>();
```

### Constant Mem. Parameter Speedup

#### Problem size

- n=1000, step=10000
- n=1000, step=10000
- n=3000, step=10000

### Speedup

- CC 1.3: 1.015
- CC 2.0: 1.016
- CC 3.0: 0.971

#### Performance

- Minimal perf. impact
- May be useful for very short kernels that are often invoked

#### Benefit

 Less shared memory used on CC 1.3 devices

### Using the RSQRTF Instruction

- Slowest kernel operation
  - Computing one over the square root is very slow
  - GPU has slightly imprecise but fast 1/sqrt instruction
     (frequently used in graphics code to calculate inverse of distance to a point)
- IEEE floating-point accuracy compliance
  - CC 1.x is not entirely compliant
  - CC 2.x and above are compliant but also offer faster non-compliant instructions

### Using the RSQRT Instruction

```
for (i = 0; i < nbodies; i++) {
  for (j = 0; j < nbodies; j++) {
    if (i != j) {
     dx = body[j].posx - px;
     dy = body[j].posy - py;
     dz = body[j].posz - pz;
     dsq = dx*dx + dy*dy + dz*dz;
     dinv = 1.0f / sqrtf(dsq + epssq);
     dinv = rsqrtf(dsq + epssq);
      scale = body[j].mass * dinv * dinv * dinv;
      ax += dx * scale;
      ay += dy * scale;
      az += dz * scale;
```

## RSQRT Speedup

#### Problem size

- n=100000, step=1
- n=100000, step=1
- n=300000, step=1

### Speedup

- CC 1.3: 0.99

- CC 2.0: 1.83

- CC 3.0: 1.64

#### Performance

- Little change for CC 1.3
  - Compiler automatically uses less precise RSQRTF as most FP ops are not fully precise anyhow
- 83% speedup for CC 2.0
  - Over entire application
  - Compiler defaults to precise instructions
  - Explicit use of RSQRTF indicates imprecision okay

### Using 2 Loops to Avoid If Statement

- "if (i != j)" creates code divergence
  - Break loop into two loops to avoid if statement

```
for (j = 0; j < nbodies; j++) {
   if (i != j) {
      dx = body[j].posx - px;
      dy = body[j].posy - py;
      dz = body[j].posz - pz;
      dsq = dx*dx + dy*dy + dz*dz;
      dinv = rsqrtf(dsq + epssq);
      scale = body[j].mass * dinv * dinv * dinv;
      ax += dx * scale;
      ay += dy * scale;
      az += dz * scale;
   }
}</pre>
```

## Using 2 Loops to Avoid If Statement

```
for (j = 0; j < i; j++) {
 dx = body[j].posx - px;
 dy = body[j].posy - py;
 dz = body[i].posz - pz;
 dsq = dx*dx + dy*dy + dz*dz;
 dinv = rsqrtf(dsq + epssq);
  scale = body[j].mass * dinv * dinv * dinv;
 ax += dx * scale:
 ay += dy * scale;
 az += dz * scale;
for (j = i+1; j < nbodies; j++) {
 dx = body[j].posx - px;
 dy = body[j].posy - py;
 dz = body[j].posz - pz;
 dsq = dx*dx + dy*dy + dz*dz;
 dinv = rsqrtf(dsq + epssq);
  scale = body[j].mass * dinv * dinv * dinv;
 ax += dx * scale;
  ay += dy * scale;
 az += dz * scale;
```

## Loop Duplication Speedup

### Problem size

- n=100000, step=1
- n=100000, step=1
- n=300000, step=1

### Speedup

- CC 1.3: 0.55

- CC 2.0: 1.00

- CC 3.0: 1.00

### Performance

- No change for 2.0 & 3.0
  - Divergence moved to loop
- 45% slowdown for CC 1.3
  - Unclear reason

#### Discussion

- Not a useful optimization
- Code bloat
- A little divergence is okay (only 1 in 3125 iterations)

## **Blocking using Shared Memory**

- Code is memory bound
  - Each warp streams in all bodies' masses and positions
- Use shared memory in inner loop
  - Read block of mass & position info into shared mem
  - Requires barriers (fast hardware barrier within SM)
- Advantage
  - A lot fewer main memory accesses
  - Remaining main memory accesses are fully coalesced (due to usage of scalar arrays)

## **Blocking using Shared Memory**

```
shared float posxs[threads], posys[threads], poszs[...], masss[...];
i = 0;
for (j1 = 0; j1 < nbodiesd; j1 += THREADS) { // first part of loop</pre>
 idx = tid + i1;
 if (idx < nbodiesd) { // each thread copies 4 words (fully coalesced)</pre>
   posxs[id] = posxd[idx]; posys[id] = posyd[idx];
   poszs[id] = poszd[idx]; masss[id] = massd[idx];
  syncthreads(); // wait for all copying to be done
 bound = min(nbodiesd - j1, THREADS);
 for (j2 = 0; j2 < bound; j2++, j++) { // second part of loop}
   if (i != j) {
     dx = posxs[j2] - px; dy = posys[j2] - py; dz = poszs[j2] - pz;
     dsq = dx*dx + dy*dy + dz*dz;
     dinv = rsqrtf(dsq + epssqd);
      scale = masss[j2] * dinv * dinv * dinv;
     ax += dx * scale; ay += dy * scale; az += dz * scale;
   syncthreads(); // wait for all force calculations to be done
```

## **Blocking Speedup**

### Problem size

- n=100000, step=1
- n=100000, step=1
- n=300000, step=1

### Speedup

- CC 1.3: 3.7
- CC 2.0: 1.1
- CC 3.0: 1.6

### Performance

- Great speedup for CC 1.3
- Some speedup for others
  - Has hardware data cache

### Discussion

- Very important optimization for memory bound code
- Even with L1 cache

# **Loop Unrolling**

- CUDA compiler
  - Generally good at unrolling loops with fixed bounds
  - Does not unroll inner loop of our example code
- Use pragma to unroll (and pad arrays)

```
#pragma unroll 8
for (j2 = 0; j2 < bound; j2++, j++) {
   if (i != j) {
      dx = posxs[j2] - px;      dy = posys[j2] - py;      dz = poszs[j2] - pz;
      dsq = dx*dx + dy*dy + dz*dz;
      dinv = rsqrtf(dsq + epssqd);
      scale = masss[j2] * dinv * dinv * dinv;
      ax += dx * scale;      ay += dy * scale;      az += dz * scale;
   }
}</pre>
```

## Loop Unrolling Speedup

### Problem size

- n=100000, step=1
- n=100000, step=1
- n=300000, step=1

### Speedup

- CC 1.3: 1.07
- CC 2.0: 1.16
- CC 3.0: 1.07

### Performance

- Insignificant speedup
- All three GPUs

#### Discussion

- Can be useful
- May increase register
  usage, which may lower
  maximum number of
  threads per block and
  result in slowdown

### CC 2.0 Absolute Performance

- Problem size
  - n=100000, step=1
- Runtime
  - 612 ms
- FP operations
  - 326.7 GFlop/s
- Main mem throughput
  - $1.035 \, GB/s$

- Not peak performance
  - Only 32% of 1030 GFlop/s
    - Peak assumes FMA every cycle
  - 3 sub (1c), 3 fma (1c), 1 rsqrt (8c), 3 mul (1c), 3 fma (1c) =20c for 20 Flop
  - 63% of realistic peak of 515.2
     GFlop/s
    - Assumes no non-FP operations
  - With int ops = 31c for 20 Flop
  - 99% of actual peak of 330.45
     GFlop/s

# Eliminating the If Statement

- Algorithmic optimization
  - Potential softening parameter avoids division by zero
  - If-statement is not necessary and can be removed
    - Eliminates thread divergence

## If Elimination Speedup

- Problem size
  - n=100000, step=1
  - n=100000, step=1
  - n=300000, step=1
- Speedup
  - CC 1.3: 1.38
  - CC 2.0: 1.54
  - CC 3.0: 1.64

- Performance
  - Large speedup
  - All three GPUs
- Discussion
  - No thread divergence
  - Allows compiler to schedule code much better

### Rearranging Terms

- Generated code is suboptimal
  - Compiler does not emit as many fused multiplyadd (FMA) instructions as it could
  - Rearrange terms in expressions to help compiler
    - Need to check generated assembly code

```
for (j2 = 0; j2 < bound; j2++, j++) {
   dx = posxs[j2] - px;   dy = posys[j2] - py;   dz = poszs[j2] - pz;
   dsq = dx*dx + dy*dy + dz*dz;
   dinv = rsqrtf(dsq + epssqd);
   dsq = dx*dx + (dy*dy + (dz*dz + epssqd));
   dinv = rsqrtf(dsq);
   scale = masss[j2] * dinv * dinv * dinv;
   ax += dx * scale;   ay += dy * scale;   az += dz * scale;
}</pre>
```

# FMA Speedup

- Problem size
  - n=100000, step=1
  - n=100000, step=1
  - n=300000, step=1
- Speedup
  - CC 1.3: 1.03
  - CC 2.0: 1.05
  - CC 3.0: 1.06

- Performance
  - Small speedup
  - All three GPUs

- Discussion
  - Seemingly needless transformations may make a difference

## Higher Unroll Factor

- Problem size
  - n=100000, step=1
  - n=100000, step=1
  - n=300000, step=1
- Speedup
  - CC 1.3: 1.01
  - CC 2.0: 1.04
  - CC 3.0: 0.93

- Unroll 128 times
  - Avoid looping overhead
  - Now that there are no ifs
- Performance
  - Little speedup/slowdown
- Discussion
  - Carefully choose unroll factor (manually tune)

## Compiler Flags

- Problem size
  - n=100000, step=1
  - n=100000, step=1
  - n=300000, step=1
- Speedup
  - CC 1.3: 1.00
  - CC 2.0: 1.18
  - CC 3.0: 1.15

- -use\_fast\_math
  - "-ftz=true" suffices(flush denormals to zero)
  - Makes SP FP operations faster except on CC 1.3
- Performance
  - Significant speedup
- Discussion
  - Use faster but less precise operations when prudent

### Final Absolute Performance

- CC 2.0 Fermi GTX 480
  - Problem size
    - n=100000, step=1
  - Runtime
    - 296.1 ms
  - FP operations
    - 675.6 GFlop/s (SP)
    - 66% of peak performance
    - 261.1 GFlops/s (DP)
  - Main mem throughput
    - 2.139 GB/s

- CC 3.0 Kepler GTX 680
  - Problem size
    - n=300000, step=1
  - Runtime
    - 1073 ms
  - FP operations
    - 1677.6 GFlop/s (SP)
    - 54% of peak performance
    - 88.7 GFlops/s (DP)
  - Main mem throughput
    - 5.266 GB/s

## **Hybrid Execution**

- CPU always needed for program launch and I/O
  - CPU much faster on serial program segments
- GPU 10 times faster than CPU on parallel code
  - Running 10% of problem on CPU is hardly worthwhile
  - Complicates programming and requires data transfer
    - Best CPU data structure is often not best for GPU
- PCIe bandwidth much lower than GPU bandwidth
  - 1.6 to 6.5 GB/s versus 192 GB/s
  - But can send data while CPU & GPU are computing
  - Merging CPU and GPU on same die (e.g., AMD's Fusion APU) makes finer grain switching possible

### Summary

- Step-by-step porting and tuning of CUDA code
  - Example: n-body simulation
- GPUs have very powerful hardware
  - But only exploitable with some code
  - Harder to program and optimize than CPU hardware