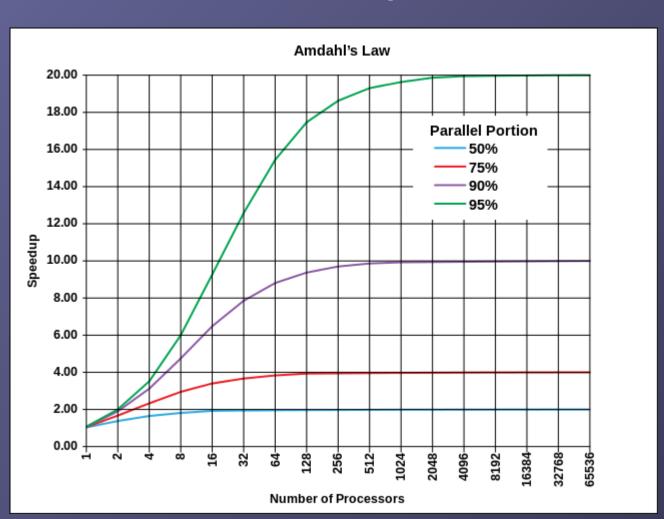
Parallel Computing

Some basic ideas

Amdahl's Law (Gene Amdahl 1967)



Evolution according to Amdahl's law of the theoretical speedup of the execution of a program in function of the number of processors executing it, for different values of p. The speedup is limited by the serial part of the program. For example, if 95% of the program can be parallelized, the theoretical maximum speedup using parallel computing would be 20 times.

By Daniels220 at English Wikipedia - Own work based on: File:AmdahlsLaw.png, CC BY-SA 3.0, https://commons.wikimedia.org/w/index.php?curid=6678551

Calculate Amdahl's Law:

Let X be the part of my program (in terms of computing time) which can be parallelised. The sequential computing time Tseq is normalized to unity (1), and can be expressed as:

Tseq =
$$1 = X + (1-X)$$

The parallel computing time Tpar under ideal conditions (ideal load balancing, ultrafast communication):

**Tpar =
$$X/p + (1-X)$$** with processor number (core number) p

Then the speed-up of the program S = Tseq / Tpar:

$$S = 1 / (1-X+X/p)$$
; Note: Tpar/Tseq = 1/S (sometimes also plotted)

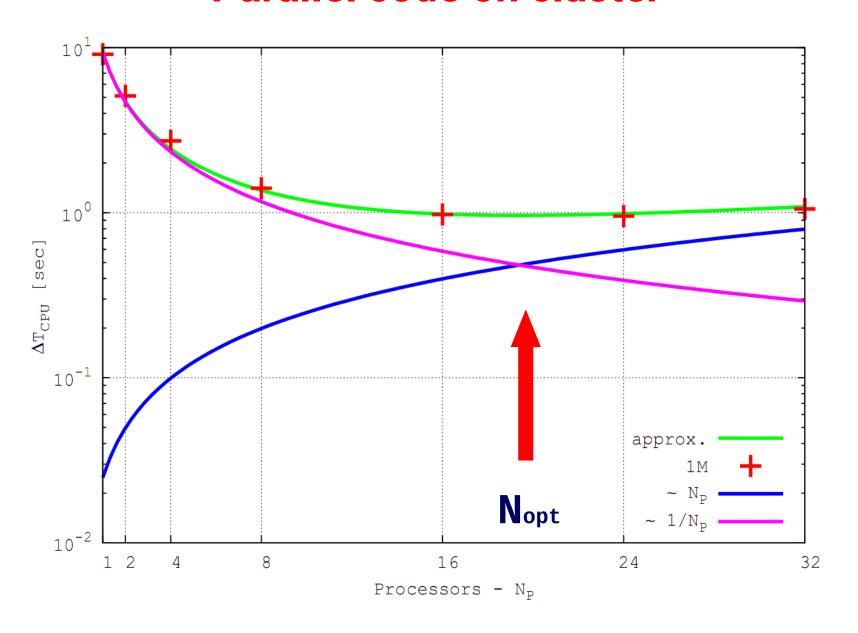
Note the limit if p is very large: S = 1/(1-X). And if $X \sim 1$: $S \sim p$

With communication overhead:

Tpar =
$$X/p + (1-X) + Tcomm$$
 \rightarrow $S = 1 / (1-X+X/p+Tcomm)$

If Tcomm independent of p we have for large p: S = 1 / (1-X + Tcomm) = const.

Parallel code on cluster



Strong and Soft Scaling

- Strong Scaling: Fixed Problem size, increase p
- Soft Scaling: Increase Problem size, increase p (constant amount of work per processing element)

Ansatz for Soft Scaling:

- \rightarrow Tseq = p = p (X + (1-X))
- \rightarrow Tpar = X + p (1-X)
- \Rightarrow S = Tseq/Tpar = p / (X+p (1-X)) If X~1: S = p; Tpar = X = const.

ΦGPU - NBODY Code

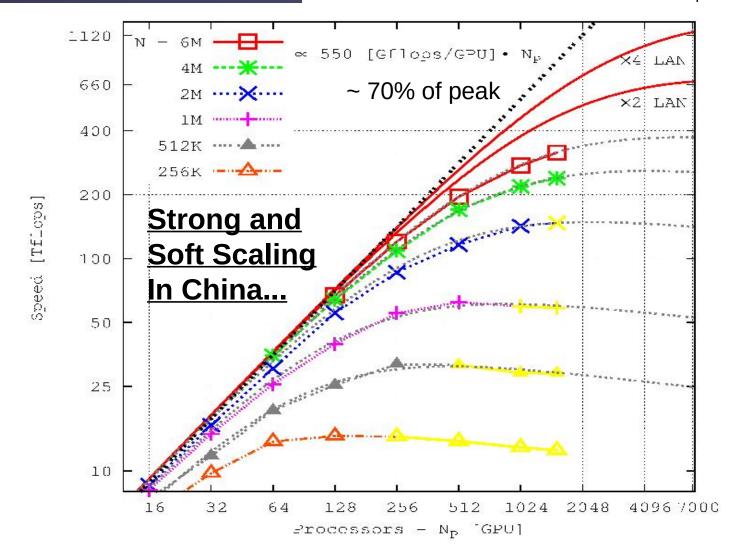


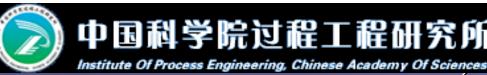
National Astronomical Observatories, CAS

350 Teraflop/s 1600 GPUs . 440 cores = 704.000 GPU-Cores

Using Mole-8.5 of IPE/CAS Beijing

Berczik et al. 2013





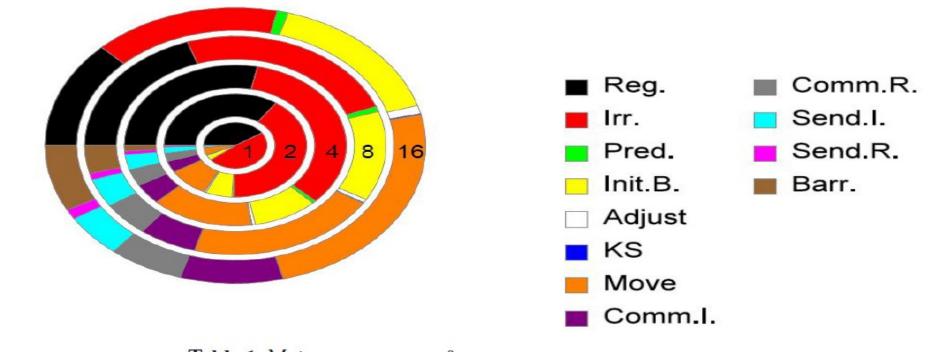
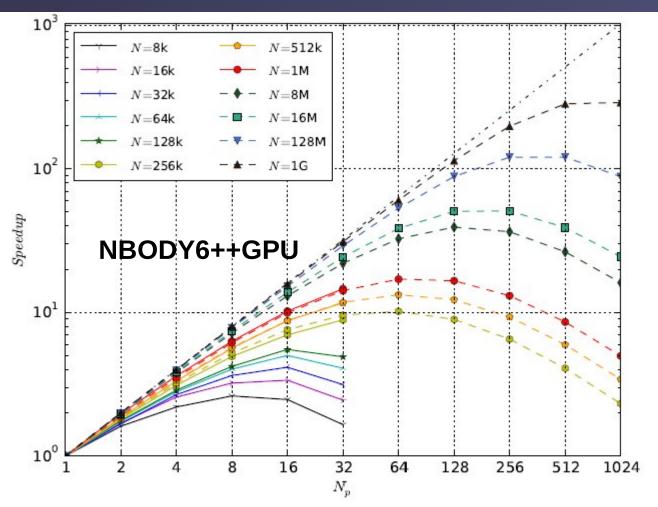


Table 1 Main components of NBODY6++

Description	Timing	Expected scaling		From the Land
	variable	variable N N_p Fitting value	Fitting value [sec]	
Regular force computation	$T_{ m reg}$	$\mathcal{O}(N_{\mathrm{reg}} \cdot N)$	$\mathcal{O}(N_p^{-1})$	$(2.2 \cdot 10^{-9} \cdot N^{2.11} + 10.43) \cdot N_p^{-1}$
Irregular force computation	$T_{ m irr}$	$\mathcal{O}(N_{\mathrm{irr}} \cdot \langle N_{nb} \rangle)$	$\mathcal{O}(N_p^{-1})$	$(3.9 \cdot 10^{-7} \cdot N^{1.76} - 16.47) \cdot N_p^{-1}$
Prediction	$T_{ m pre}$	$\mathcal{O}(N^{kn_p})$	$\mathcal{O}(N_p^{-kp_p})$	$(1.2 \cdot 10^{-6} \cdot N^{1.51} - 3.58) \cdot N_p^{-0.5}$
Data moving	$T_{ m mov}$	$\mathcal{O}(N^{kn_{m1}})$	$\mathcal{O}(1)$	$2.5 \cdot 10^{-6} \cdot N^{1.29} - 0.28$
MPI communication (regular)	$T_{ m mcr}$	$\mathcal{O}(N^{kn_{cr}})$	$\mathcal{O}(kp_{cr} \cdot \frac{N_p-1}{N_p})$	$(3.3 \cdot 10^{-6} \cdot N^{1.18} + 0.12)(1.5 \cdot \frac{N_p - 1}{N_p})$
MPI communication (irregular)	$T_{ m mci}$	$\mathcal{O}(N^{kn_{ci}})$	$\mathcal{O}(kp_{ci} \cdot \frac{N_p-1}{N_p})$	$(3.6 \cdot 10^{-7} \cdot N^{1.40} + 0.56)(1.5 \cdot \frac{N_p-1}{N_p})$
Synchronization	$T_{ m syn}$	$\mathcal{O}(N^{kn_s})$	$\mathcal{O}(N_p^{kp_s})$	$(4.1 \cdot 10^{-8} \cdot N^{1.34} + 0.07) \cdot N_p$
Sequential parts on host	$T_{ m host}$	$\mathcal{O}(N^{kn_h})$	$\mathcal{O}(1)$	$4.4 \cdot 10^{-7} \cdot N^{1.49} + 1.23$



Huang, Berczik, Spurzem, Res. Astron. Astroph. 2016, 16, 11.

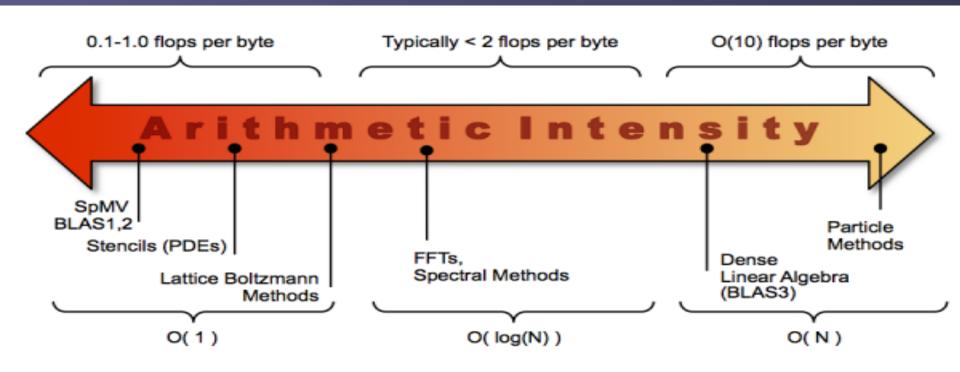
Fig. 2 The speed-up (S) of NBODY6++ as a function of particle number (N) and processor number (N_p) . Solid points are the measured speed-up ratio between sequential and parallel wall-clock time, dash lines predict the performance of larger scale simulations further. The symbols used in figure have the magnitudes: $1k = 1,024, 1M = 1k^2$ and $1G = 1k^3$.

Roofline Performance Model (LBL)

http://crd.lbl.gov/departments/computer-science/PAR/research/roofline

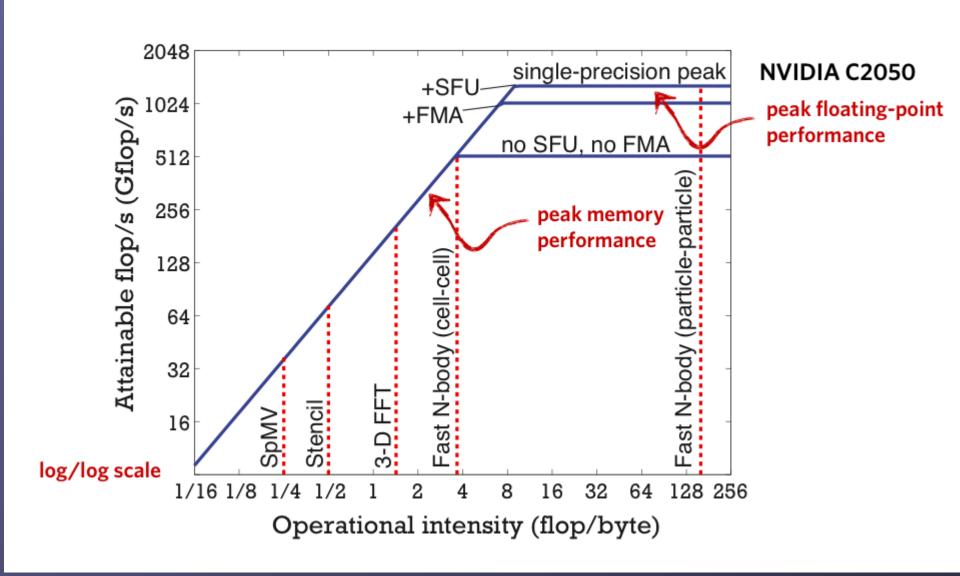
Arithmetic Intensity

The core parameter behind the Roofline model is Arithmetic Intensity. Arithmetic Intensity is the ratio of total floating-point operations to total data movement (bytes).



Roofline Performance Model (LBL)

http://lorenabarba.com/wp-content/uploads/2012/01/roofline_slide.png



Parallel Computing

Matrix Multiply and Debugging

Timing with CUDA Event API

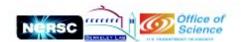
```
int main ()
                                              CUDA Event API Timer are,
     cudaEvent_t start, stop;
     float time;

    OS independent

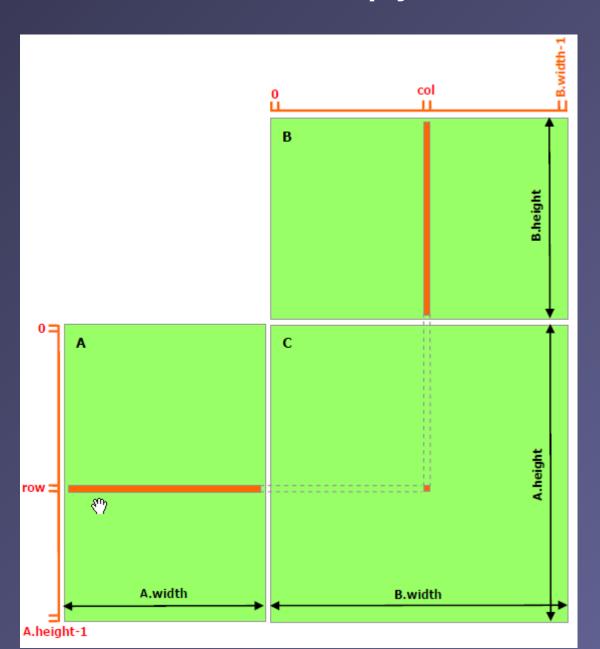
     cudaEventCreate (&start);
                                              - High resolution
     cudaEventCreate (&stop);

    Useful for timing asynchronous calls

     cudaEventRecord (start, 0);
     someKernel <<<grids, blocks, 0, 0>>> (...);
     cudaEventRecord (stop, 0);
     cudaEventSynchronize (stop); - Ensures kernel execution has completed
     cudaEventElapsedTime (&time, start, stop);
     cudaEventDestroy (start);
     cudaEventDestroy (stop);
     printf ("Elapsed time %f sec\n", time*.001);
     return 1;
                                        Standard CPU timers will not measure the
}
                                        timing information of the device.
```



Intuitive multiply

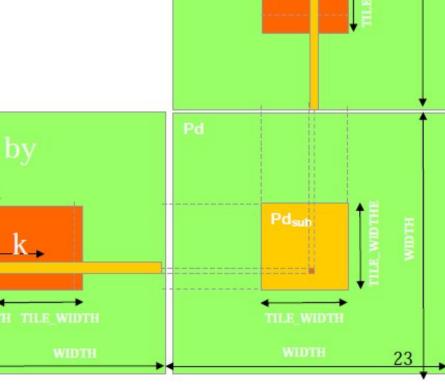


Tiled Multiply

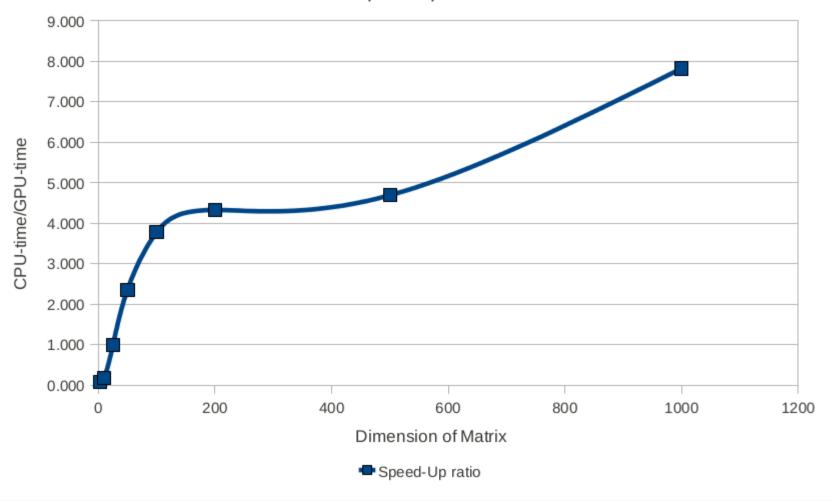
- Each block computes one square sub-matrix Pd_{sub} of size TILE_WIDTH
- Each thread computes one element of Pd_{sub}

©Wen-mei W. Hwu and David Kirk/NVIDIA,

Berkeley, January 24-25, 2011



Speed-Up Ratio
GPU speed-up over CPU



CUDA – GNU Debugger – CUDA-gdb

http://docs.nvidia.com/cuda/cuda-gdb/index.html



CUDA TOOLKIT DOCUMENTATION



CUDA Toolkit v7.5

CUDA-GDB

- ▶ 1. Introduction
- 2. Release Notes
- ⇒ 3. Getting Started

- 7. Breakpoints & Watchpoints
- ▶ 8. Inspecting Program State
- ▷ 9. Event Notifications
- ▶ 10. Automatic Error Checking
- ▶ 11. Walk-Through Examples
- ▶ 12. Advanced Settings
- A. Supported Platforms
- B. Known Issues

CUDA-GDB

1. Introduction

This document introduces CUDA-GDB, the NVIDIA® CUDA® debugger for Linux and Mac OS.

1.1. What is CUDA-GDB?

CUDA-GDB is the NVIDIA tool for debugging CUDA applications running on Linux and Mac. CUDA-GDB is an extension to the x86-64 port of GDB, the GNU Project debugger. The tool provides developers with a mechanism for debugging CUDA applications running on actual hardware. This enables developers to debug applications without the potential variations introduced by simulation and emulation environments.

CUDA-GDB runs on Linux and Mac OS X, 32-bit and 64-bit. CUDA-GDB is based on GDB 7.6 on both Linux and Mac OS X.

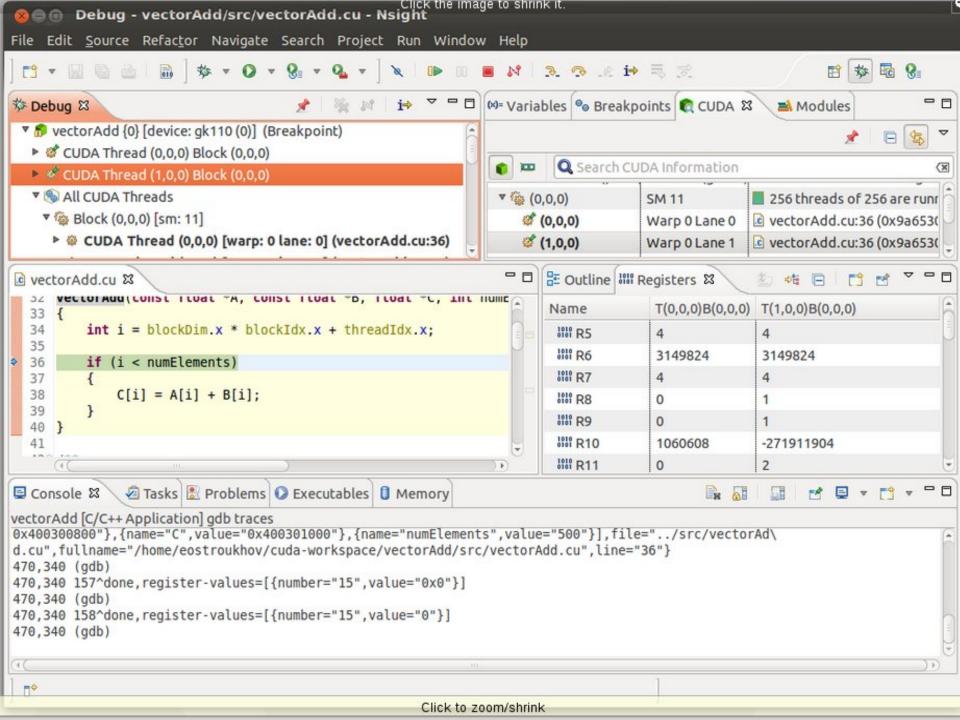
1.2. Supported Features

CUDA-GDB is designed to present the user with a seamless debugging environment that allows simultaneous debugging of both GPU and CPU code within the same application. Just as programming in CUDA C is an extension to C programming, debugging with CUDA-GDB is a natural extension to debugging with GDB. The existing GDB debugging features are inherently present for debugging the host code, and additional features have been provided to support debugging CUDA device code.

CUDA-GDB supports debugging C/C++ and Fortran CUDA applications. (Fortran debugging support is limited to 64-bit Linux operating system) All the C++ features supported by the NVCC compiler can be debugged by CUDA-GDB.

CUDA-GDB allows the user to set breakpoints, to single-step CUDA applications, and also to inspect and modify the memory and variables of any given thread running on the hardware.

CUDA-GDB (PDF) - v7.5 (older) - Last updated September 1, 2015 - Send Feedback - 📑 💟 📊 🚜 🚹 🤇



Wrapping Up 1

Exercises (CUDA Lectures in afternoon)

- 1. hello, device- first kernel call, hello world, GPU properties
- 2. add vector addition using one thread in one block only
- 3. add-index vector addition using blocks in parallel, one thread per block only.
- 4. add-parallel vector addition using all blocks and threads in parallel
- 5. dot scalar product using shared memory of one block only for reduction
- 6. dot-full scalar product using shared memory and atomic add across blocks
- 7. histo histogram using fat threads and atomic add on shared and global memory, timing
- 8. dot-perfect scalar product using fat threads, shared memory, final reduction on host.
- 9. matmul matrix multiplication with tiled access shared memory

Wrapping Up 2

Elements of CUDA C learnt:

threadId.x , blockId.x, blockDim.x, gridDim.x (threadId.y, blockId.y, blockdim.y, gridDim.y kernel<<<n,m>>> (...)
__device__ __global__
_shared__
cudaMalloc / cudaFree
cudaMemcpy / cudaMemset
cudaGetDeviceProperties
cudaEventCreate, cudaEventRecord,
cudaEventSynchronize, cudaEventElapsedTime,
cudaEventDestroy
AtomicAdd

Threads, Blocks
work with 2D grids)
kernel calls
device code
shared memory on GPU
manage global memory of GPU
copy/set to or from memory
get device properties in program

CUDA profiling atomic functions

Wrapping Up 3

What we have not yet learnt...

__constant__ cudaBindTexture fat threads for 2D and 3D stencils cudaStreamCreate, cudaStreamDestroy constant memory on GPU using texture memory thread coalescence opt. working with CUDA streams