中山大學 SUN YAT-SEN UNIVERSITY

国家超级计算广州中心 NATIONAL SUPERCOMPUTER CENTER IN GUANGZHOU

多核程序设计与实践

引言

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课程概要

- 课程目标与评分标准
- Why CUDA?
- CUDA加速效果
- 安装与项目创建

课程目标

理解多核程序设计中的重要概念

– 并行、多线程、原子操作、通信、同步机制等

掌握一种多核程序设计工具

– CUDA（Compute Unified Device Architecture)

– 能用其将现有程序并行化

– 了解CUDA程序性能优化方法

– 理解CUDA架构设计原理

课程需要

- 知识储备需要
  - 熟练使用一门编程语言（最好是C或C++）
  - 最好了解：计算机图形学、指针与内存、计算机体系结构
- 硬件需要
  - 支持CUDA的显卡（NVIDIA）

课程主要内容

- 相关知识背景补充
  - CUDA与GPGPU、C语言基础、OpenMP
  - 1-3周
- CUDA基础知识
  - GPU架构、CUDA线程、内存结构、通信同步机制、性能优化
  - 4-8周
- CUDA应用举例
  - 矩阵乘法、排序、图像高斯模糊、Ray Tracing等
  - 9、11-16周

课程评分标准

- 课程总分组成
  - 编程作业（3次） 50%
  - 期中考试 10%
  - 期末大作业 30%
  - 出勤 10%
- 编程作业评分
  - 结果正确性 40%
  - 性能 30%
  - 编程规范 10%
  - 书面报告 20%

课程评分标准

编程规范举例

– 应组织到适当文件中

– 应根据功能适当划分成函数

文件开头应包含程序说明

```
########################################
##  姓名:  XXX
##  文件说明:  **********************
##  **********************************
##  **********************************
##  **********************************
##  **********************************
########################################

#include <abc.h>

int main(){
    ...
}
```

函数开头也应包含说明

程序应适当缩进

```
########################################
##  函数:  do_something
##  函数描述:  **********************
##  **********************************
##  参数描述:
##  par1: **********************
##  par2: **********************
########################################
void do_something(par1, par2){
    for( ... ){
        if( ... ){
            ...
        }
    }
}
```

课程评分标准

- 期末大作业
  - 完成情况 50%
  - 技术难度加分 20%
    - 与完成情况相关联
  - 报告 30%
    - 书面报告、现场报告
- 其他
  - 允许讨论代码，严禁抄袭
  - 3 slip days！
    - 包括周末节假日
    - 不适用于现场报告

参考书目（文档）

E. Kandrot and J. Sanders, CUDA by Example: An Introduction to General-Purpose GPU Programming, Pearson, 2010.

- 中译版：GPU高性能编程：CUDA实战

N. Wilt, The CUDA Handbook: A Comprehensive Guide to GPU Programming, Prentice Hall, 2013.

- 中译版：CUDA专家手册：GPU编程权威指南

J. Cheng, M. Grossman, and T. McKercher, Professional CUDA C Programming, Wrox, 2014.

- 中译版：CUDA C编程权威指南

NVIDIA官方文档：

- CUDA C Programming Guide
- CUDA C Programming Best Practice Guide

课程概要

课程目标与评分标准

Why CUDA?

CUDA加速效果

安装与项目创建

Why CUDA?

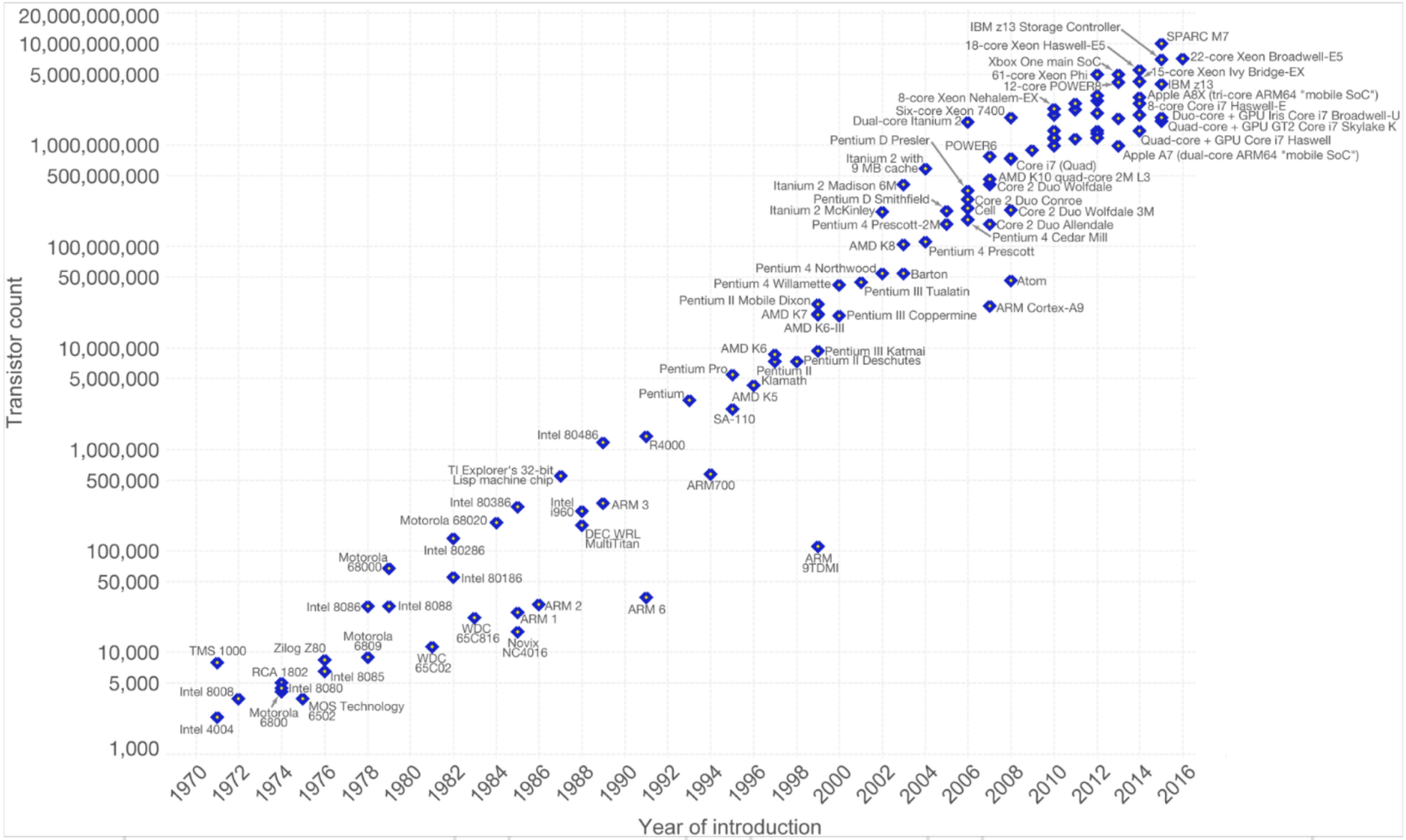
- 摩尔定律
  - 英特尔创始人之一戈登·摩尔提出：

”集成电路上可容纳的晶体管数目，
约每隔两年便会增长一倍“

  - 另一版本为18个月（由英特尔首席执行官大卫·豪斯提出）

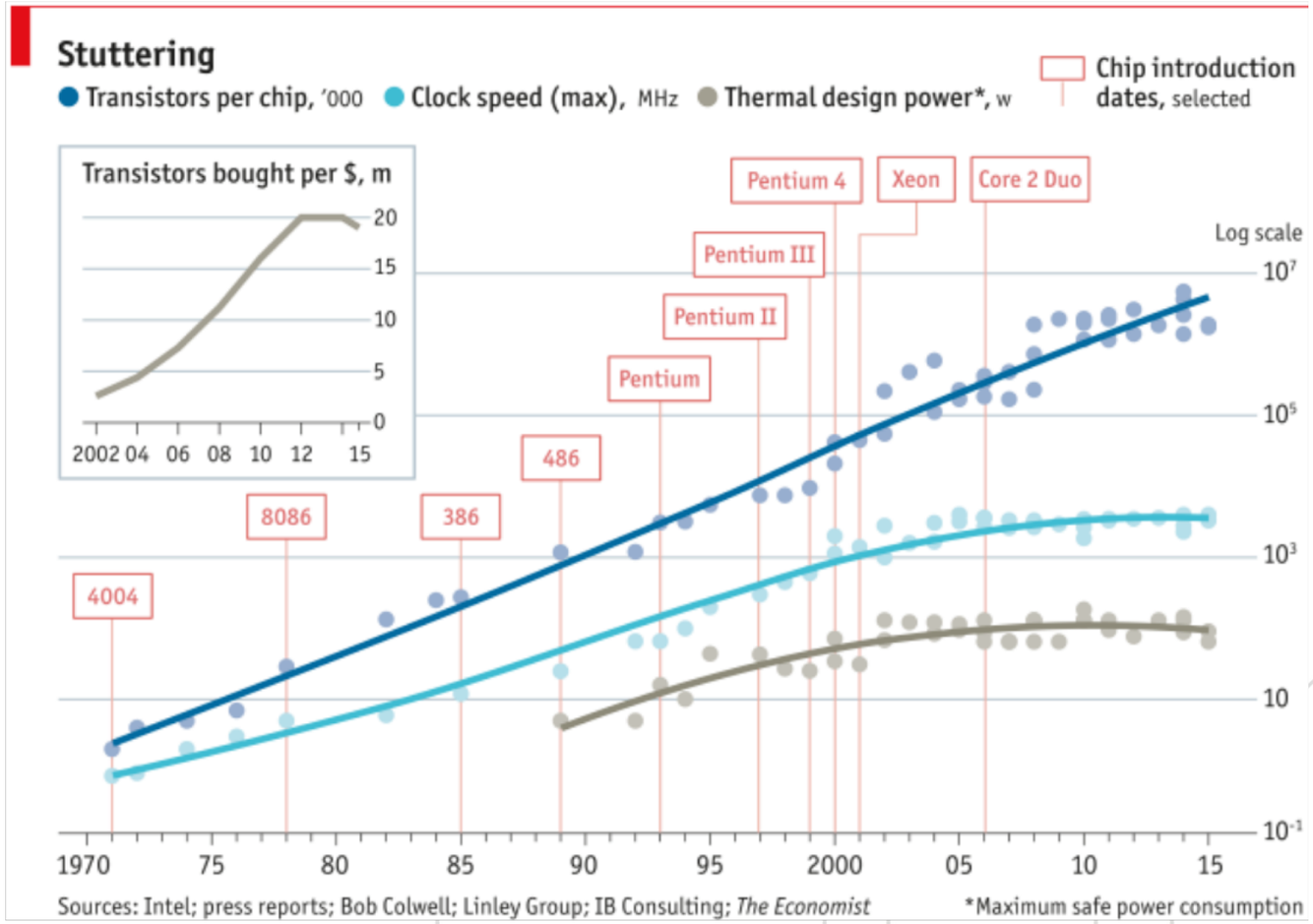
Why CUDA?

- 摩尔定律



Why CUDA?

- 摩尔定律的瓶颈
  - 晶体管数目≠频率



摩尔定律还能持续多久？

- 2021/2025年假说
- 量子穿隧效应

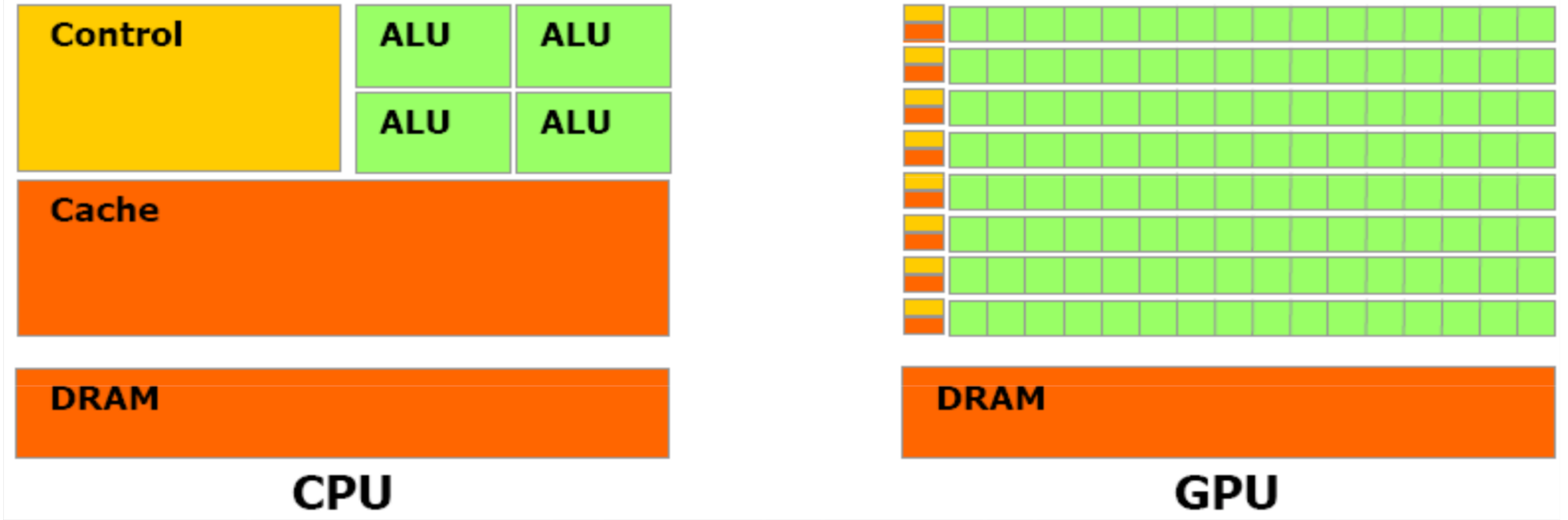
图片来源：The Economist's Technology Quartlerly

Why CUDA?

- 串行速度提升已经结束
  - 无法继续提升频率
  - 无法继续提升功耗
- 当前计算机性能提升趋势
  - 计算机没有变得更快，而是变得更宽
    - 多核CPU、GPU、超级计算机
  - 数据级别的并行
    - 同样的指令作用于多个数据
  - 线程级别的并行

Why CUDA?

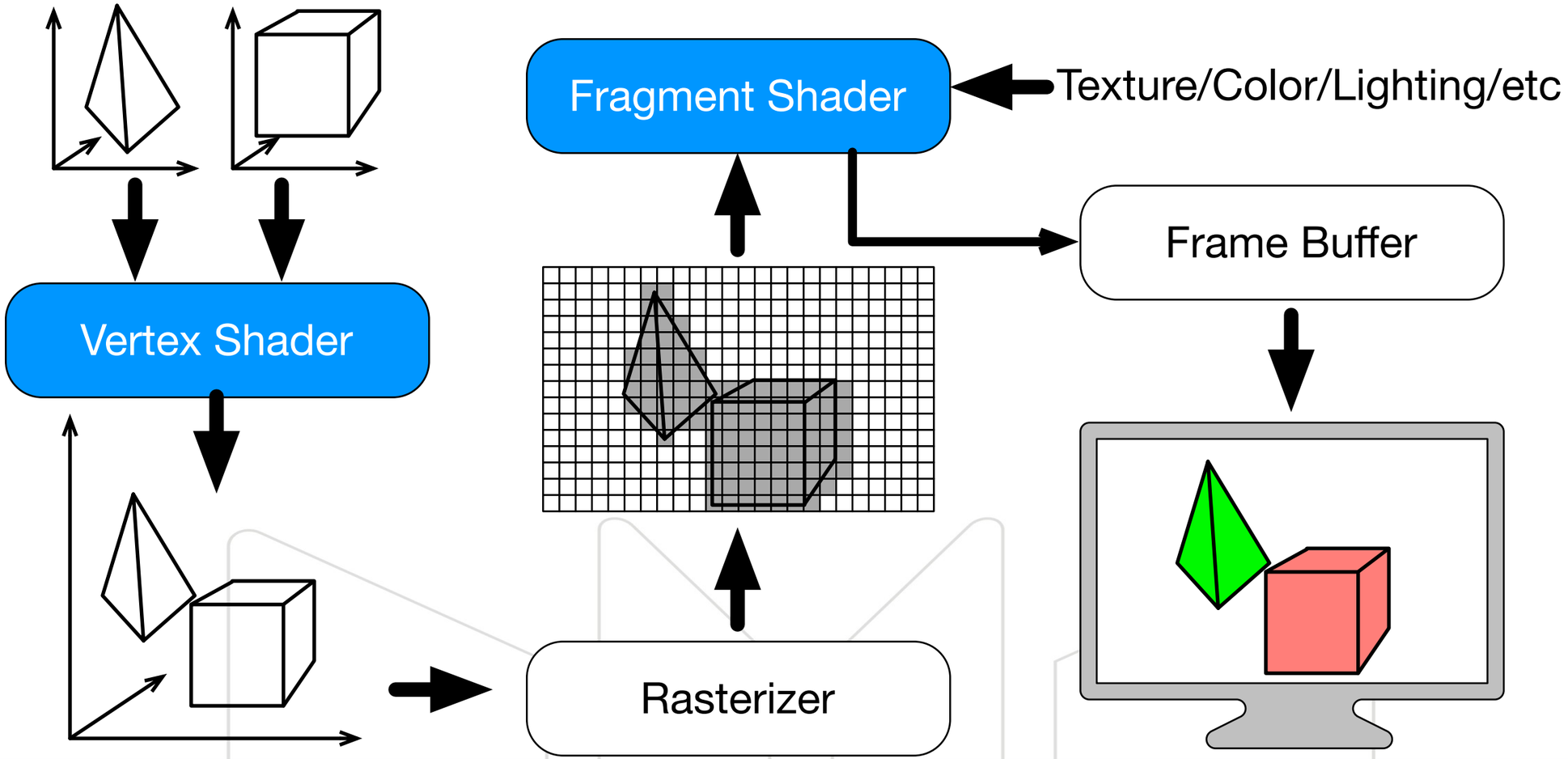
- GPGPU （General Purpose Computing for GPU)
  - GPU特征
    - 高度并行化：同样指令应用于大量数据上
    - 大量运算核心



图片来自NVIDIA

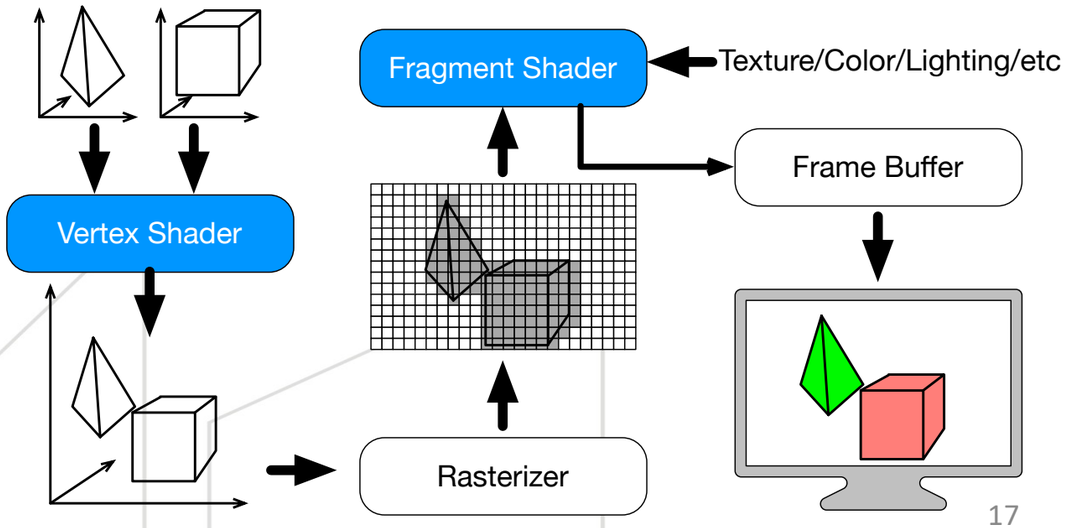
Why CUDA?

- GPGPU
  - 图形绘制简易流程



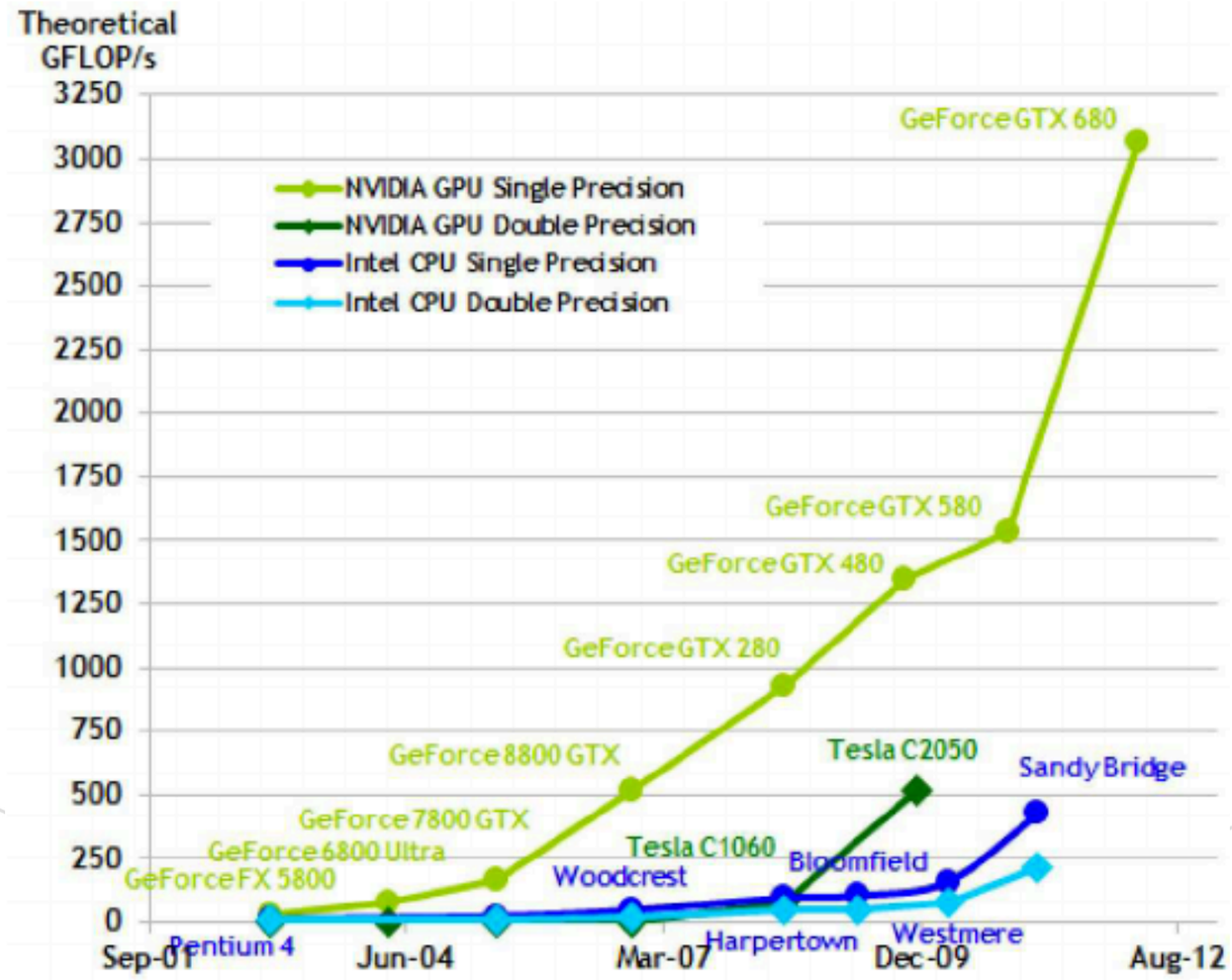
Why CUDA?

- GPGPU基本思路
  - Vertex shader 和 fragment shader 可由用户自行通过 shading language编程
  - 把封装数据封装成图形绘制库所需的数据形式传入
  - 绘制过程中通过修改shader执行用户编写的程序
    - 通常是fragment shader
  - 将结果绘制到texture中传出
  - 需要很强的图形学编程能力



Why CUDA ?

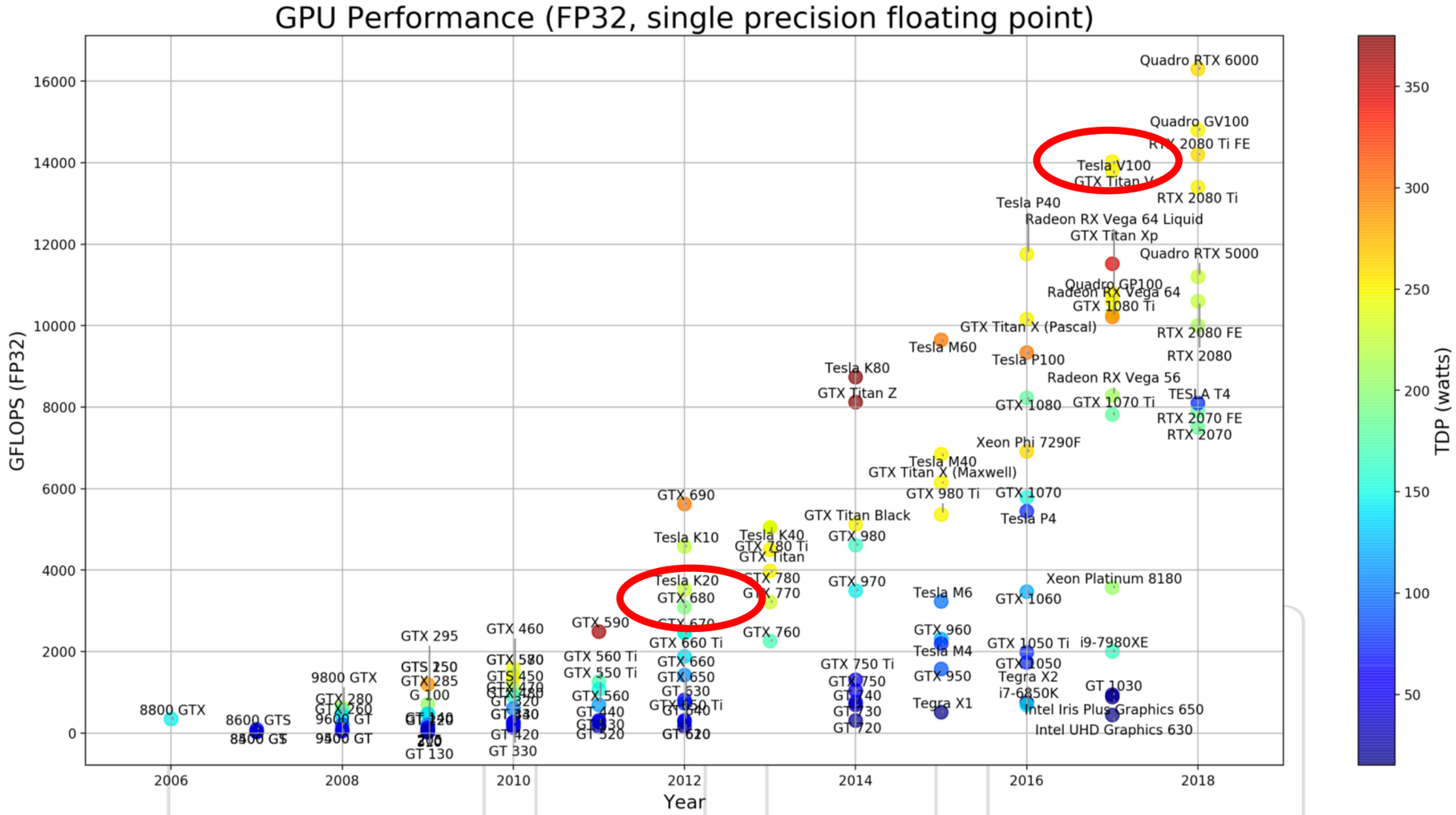
- CPU与GPU性能对比



图片来自NVIDIA

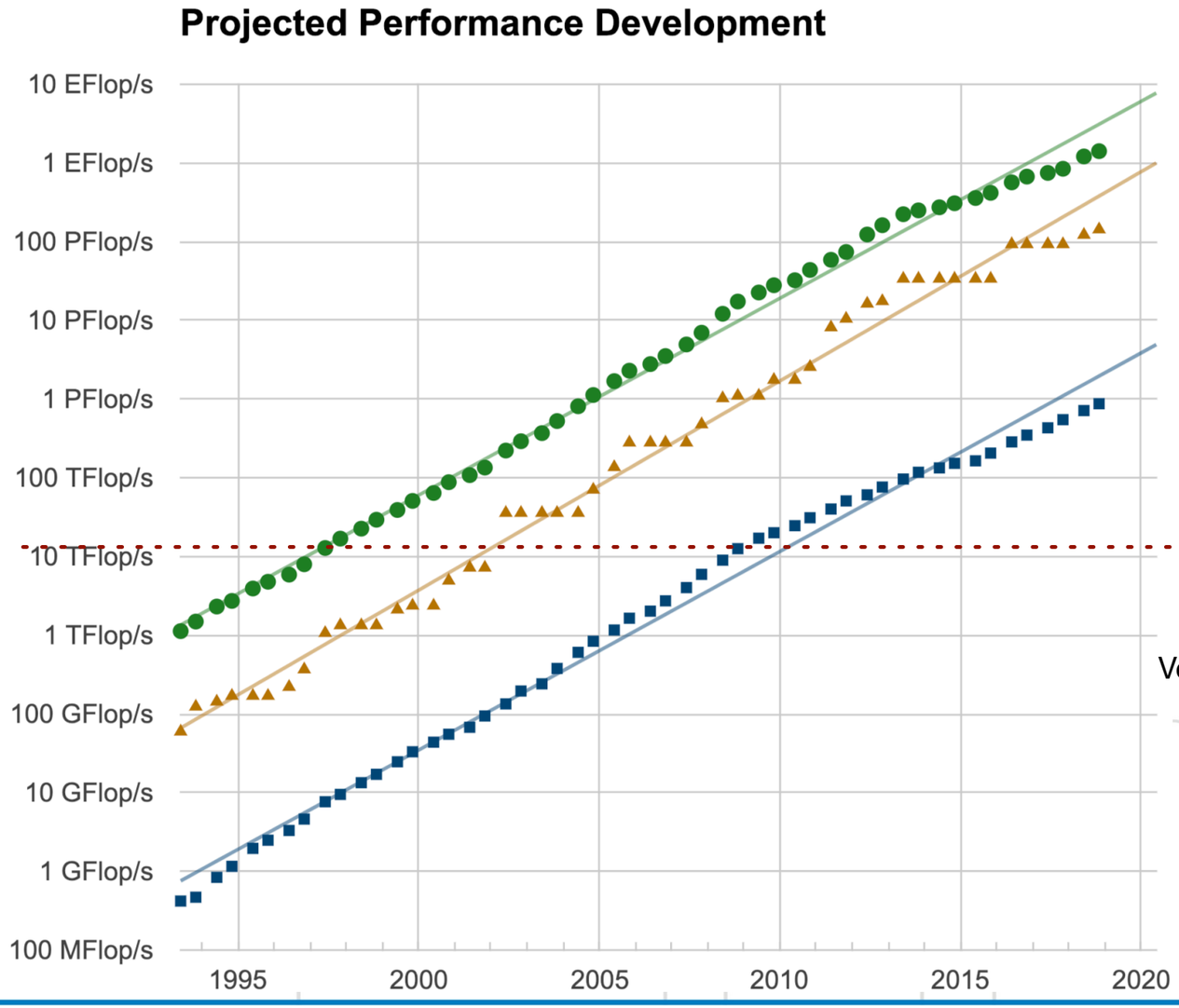
Why CUDA ?

- GPU运算速度发展



Why CUDA?

GPU与超级计算机



Volta V100 (15 TFlops/s)

图片来自https://www.top500.org/statistics/perfdevel/

Why CUDA?

CUDA vs OpenMP vs MPI

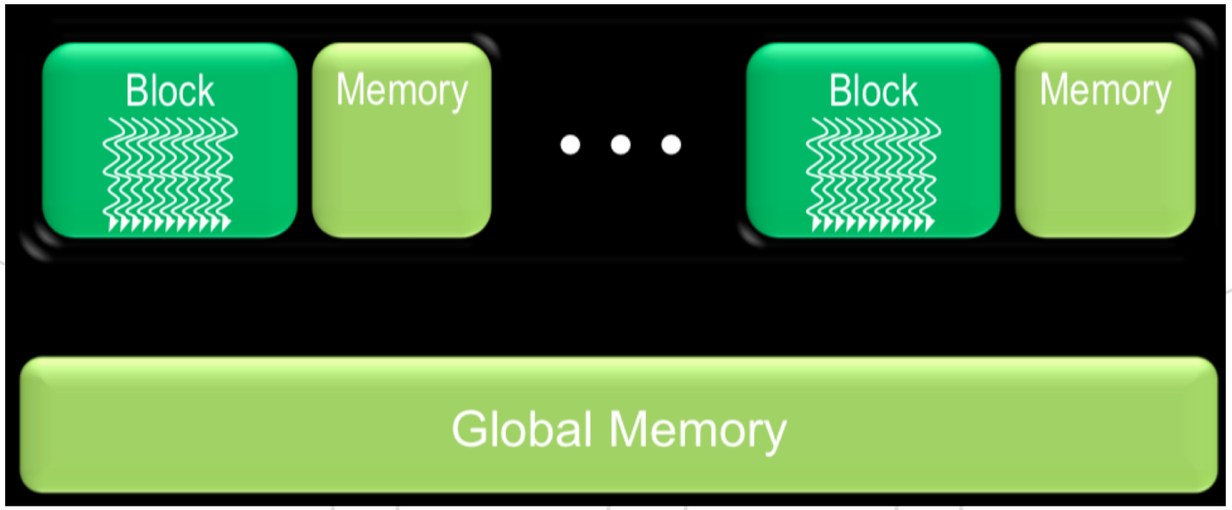
– NVIDIA显卡

– 基于GPU线程并行

Why CUDA?

CUDA vs OpenMP vs MPI

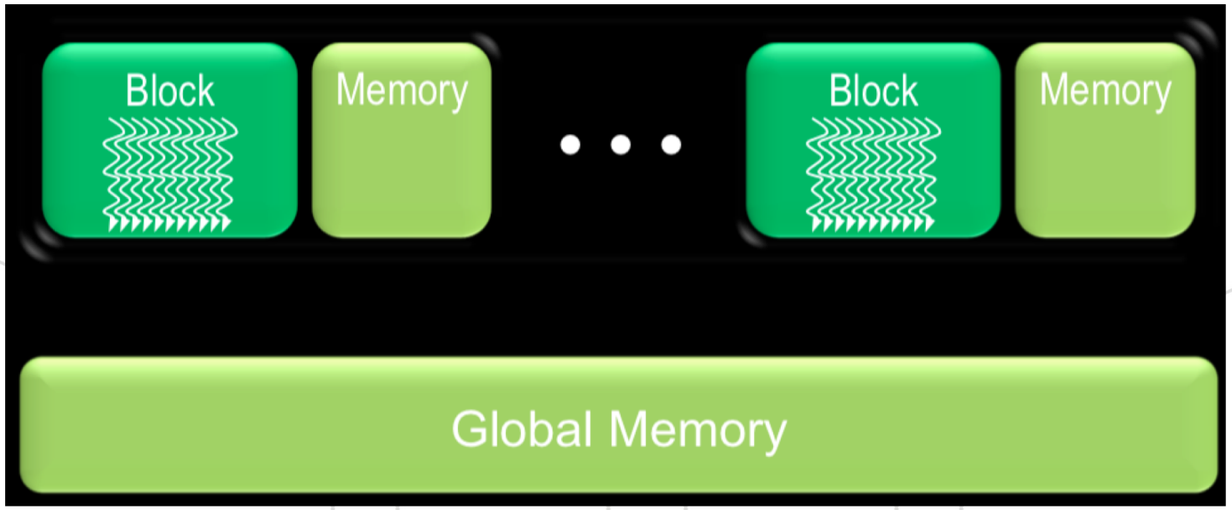
- 硬件结构
  - 图中每条波浪线代表一个线程
  - 每个block包含多个线程
    - 只有block内部线程能访问其共享内存
  - 所有线程均可访问全局存储器



图片来自NVIDIA

Why CUDA?

- CUDA vs OpenMP vs MPI
  - 硬件结构
    - 每个线程由一个CUDA core执行
    - Block中的线程以warp的形式在streaming multiprocessor上执行
      - 每个warp包含32个thread
      - warp中所有thread执行同样的指令（Single Instruction Multiple Data）



图片来自NVIDIA

Why CUDA?

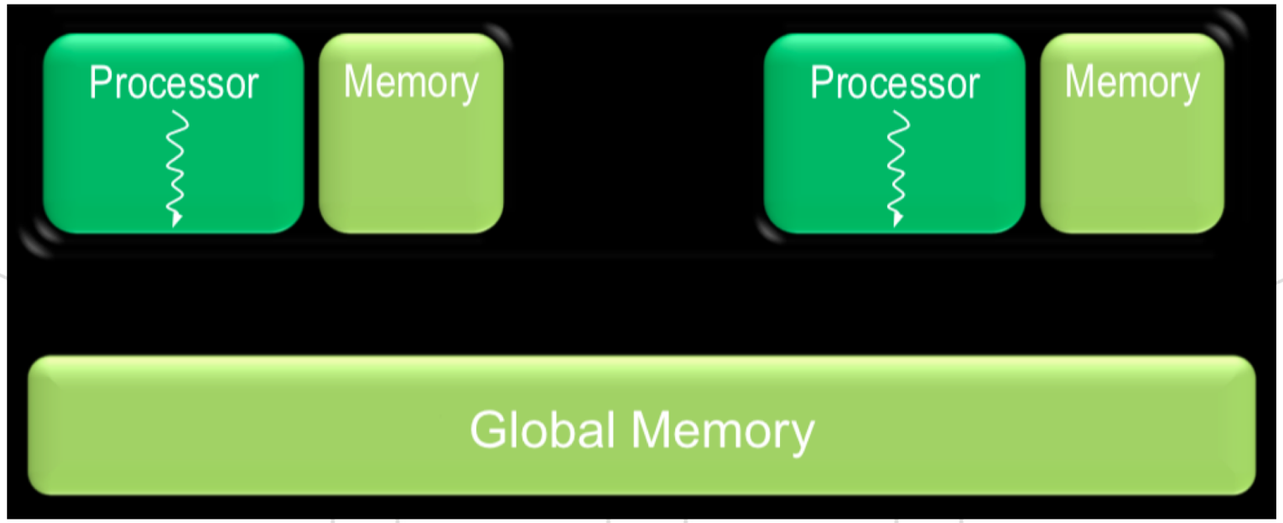
CUDA vs OpenMP vs MPI

- MP: multiprocessing
- 跨平台
- 基于共享内存的多核系统
  - 多核个人主机
  - 超级计算机（截止2017年效率并不好）

OpenMP
Enabling HPC since 1997

Why CUDA?

- CUDA vs OpenMP vs MPI
  - 硬件结构
    - 每个处理器运行一个线程
    - 每个处理器有易于访问的片上存储（on-chip memory）
    - 所有处理器共享全局存储器



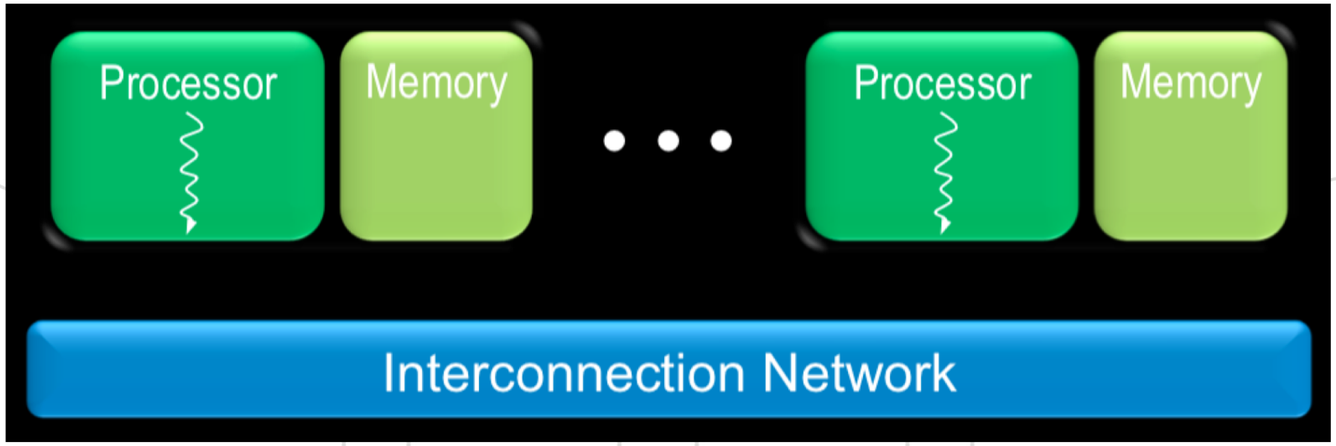
图片来自NVIDIA

Why CUDA?

- CUDA vs OpenMP vs MPI
  - MPI（Message Passing Interface）
    - 跨平台
    - 基于信息传递
    - 常用于计算机集群

Why CUDA?

- CUDA vs OpenMP vs MPI
  - 硬件结构
    - 多个处理器之间通过网络发送消息交互



图片来自NVIDIA

Why CUDA?

- CUDA vs OpenMP vs MPI
  - CUDA
    - 创建线程开销低
    - 可创建大量线程
    - 同一warp内共享指令
    - 控制流简单
  - OpenMP
    - 创建线程开销高
    - 线程数目有限
    - 线程相互间可以完全独立
    - 控制流复杂
  - MPI
    - 进程相互间可以完全独立
    - 通信成本高
    - 价格昂贵

Why CUDA?

- CUDA vs OpenCL
  - OpenCL: 跨平台的开放标准
- 生态环境：
  - CUDA：用户友好、应用广泛（目前NVIDIA投入更大）
  - OpenCL：使用稍显复杂、目前应用范围较窄
- 支持硬件：
  - CUDA：NVIDIA显卡
    - 硬件针对性更强、效率更高、对学习多核编程更有利
  - OpenCL: AMD、NVIDIA、Intel、ARM等硬件
    - 支持硬件更多、效率因硬件而异、优化因硬件而异

Why CUDA?

CUDA vs OpenCL

– OpenCL: 跨平台的开放标准

生态环境：

– CUDA：用户友好、应用广泛（目前NVIDIA投入更大）

– OpenCL：使用相应复杂、目前应用范围较窄

支持硬件：

– CUDA：NVIDIA显卡

• 硬件针对性更强、效率更高、对学习多核编程更有利

– OpenCL: AMD、NVIDIA、Intel、ARM等硬件

• 支持硬件更多、效率因硬件而异、优化因硬件而异

> “People who are really serious about software should make their own hardware.”
>
> -图灵奖得主Alan Kay

课程概要

课程目标与评分标准

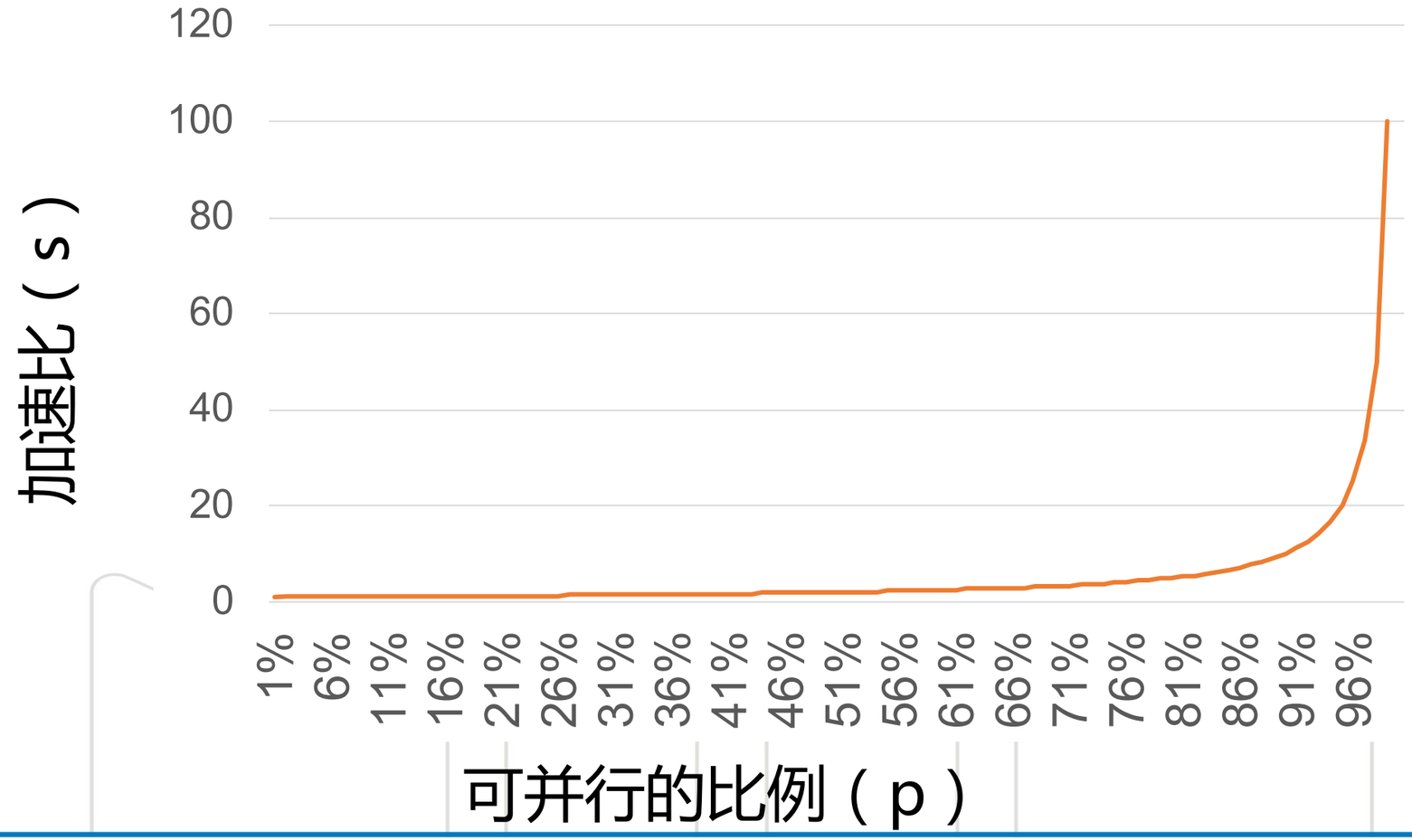
Why CUDA?

CUDA加速效果

安装与项目创建

CUDA 加速效果

- 理论效果 – Amdahl's Law
  - 程序效率受限于其可并行的比例 $s = \frac{1}{1-p}$

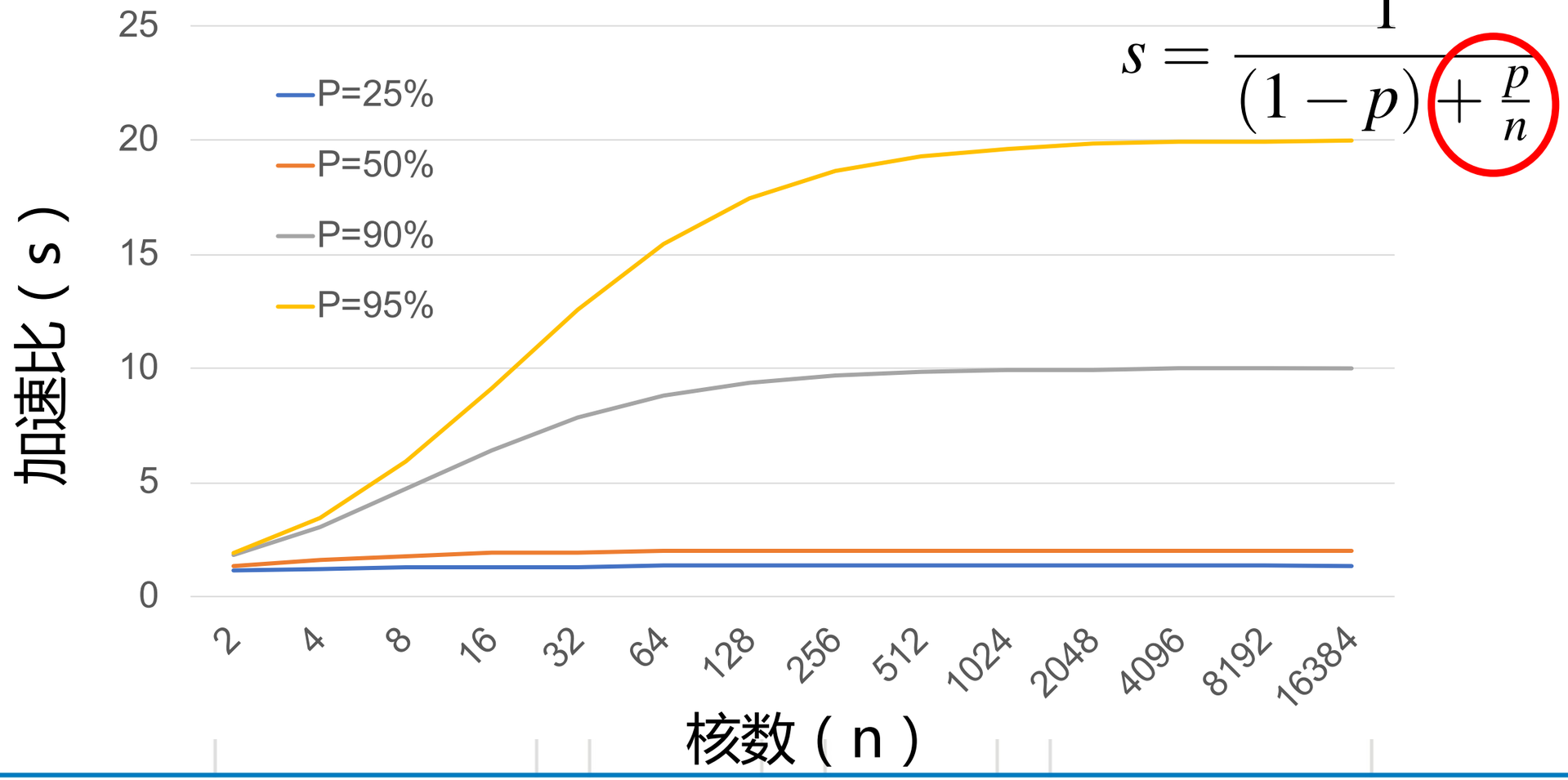


CUDA 加速效果

理论效果 – Amdahl's Law

– 程序效率受限于其可并行的比例及可供使用的核数

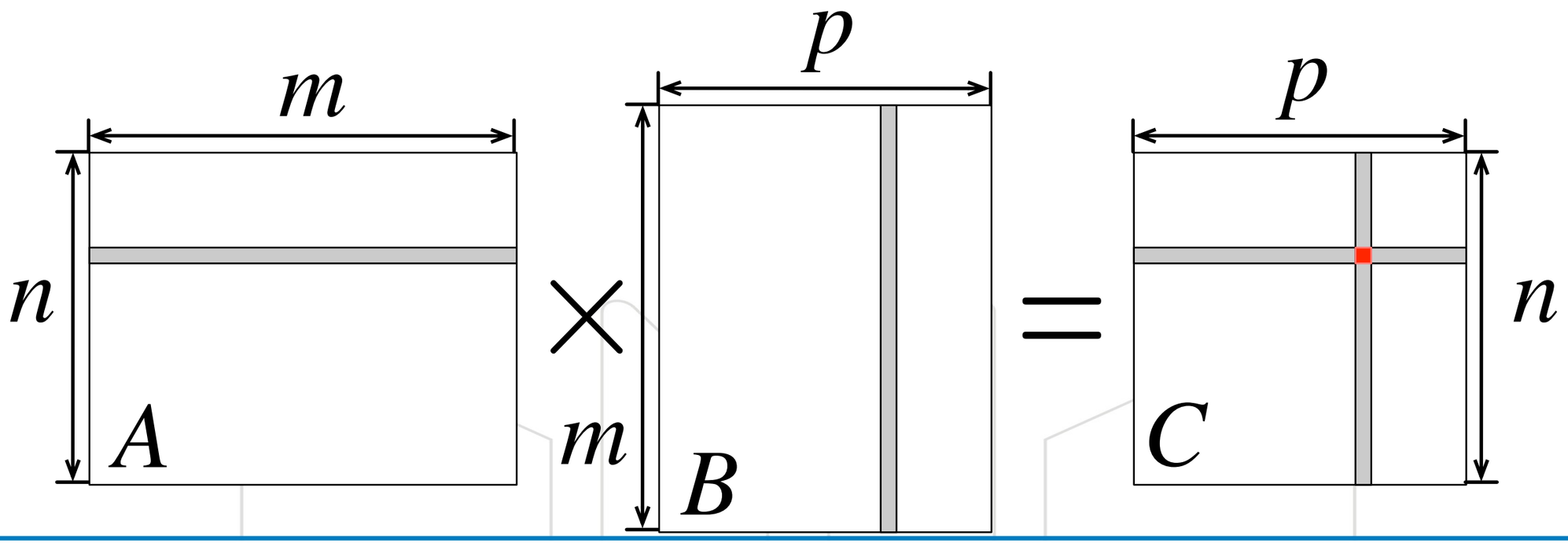
$$s = \frac{1}{(1-p) + \frac{p}{n}}$$



CUDA 加速效果

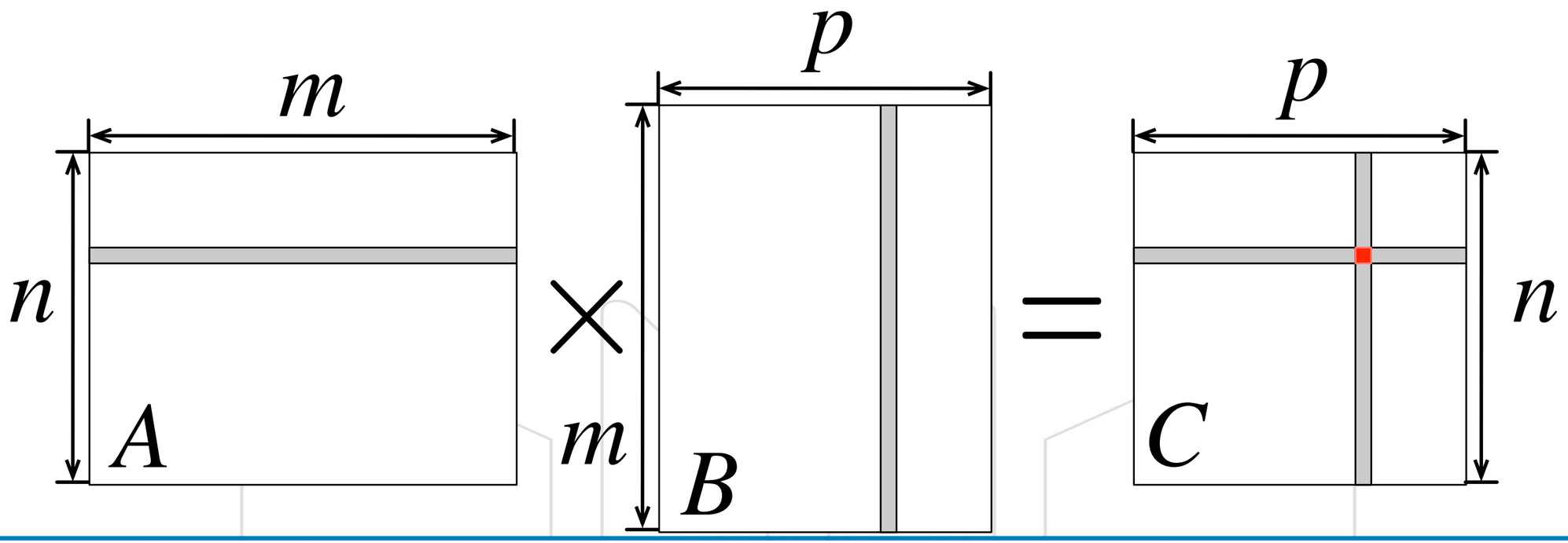
案例分析-矩阵乘法

- 对C中所有元素，计算 $C_{ij} = \sum_{k=1}^{m} A_{ik} \cdot B_{kj}$
  - 共有 $n \times p$ 次向量乘积
  - 每次向量乘积为 m 次乘法与 $m - 1$ 次加法



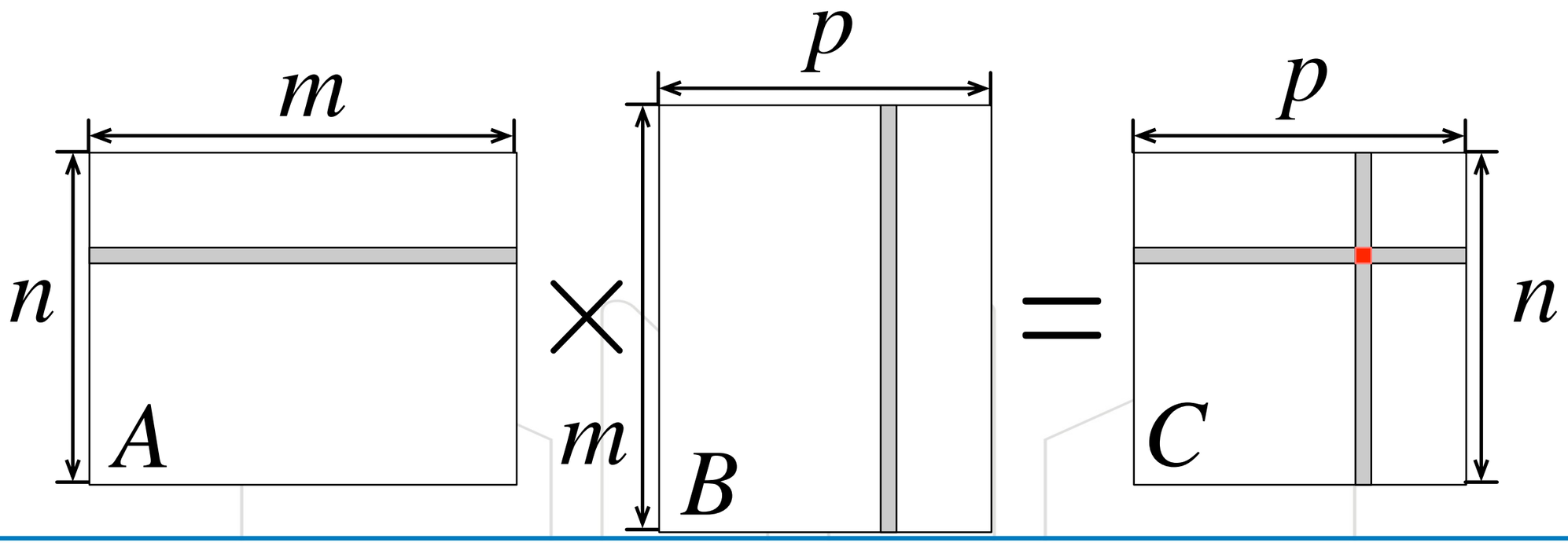
CUDA 加速效果

- 案例分析-矩阵乘法
  - 策略1：
    - 创建 $n \times p$ 个线程，每个计算一个向量点积
    - 当 $n \times p$ 大于CUDA计算核心数目时，GPU保持满载



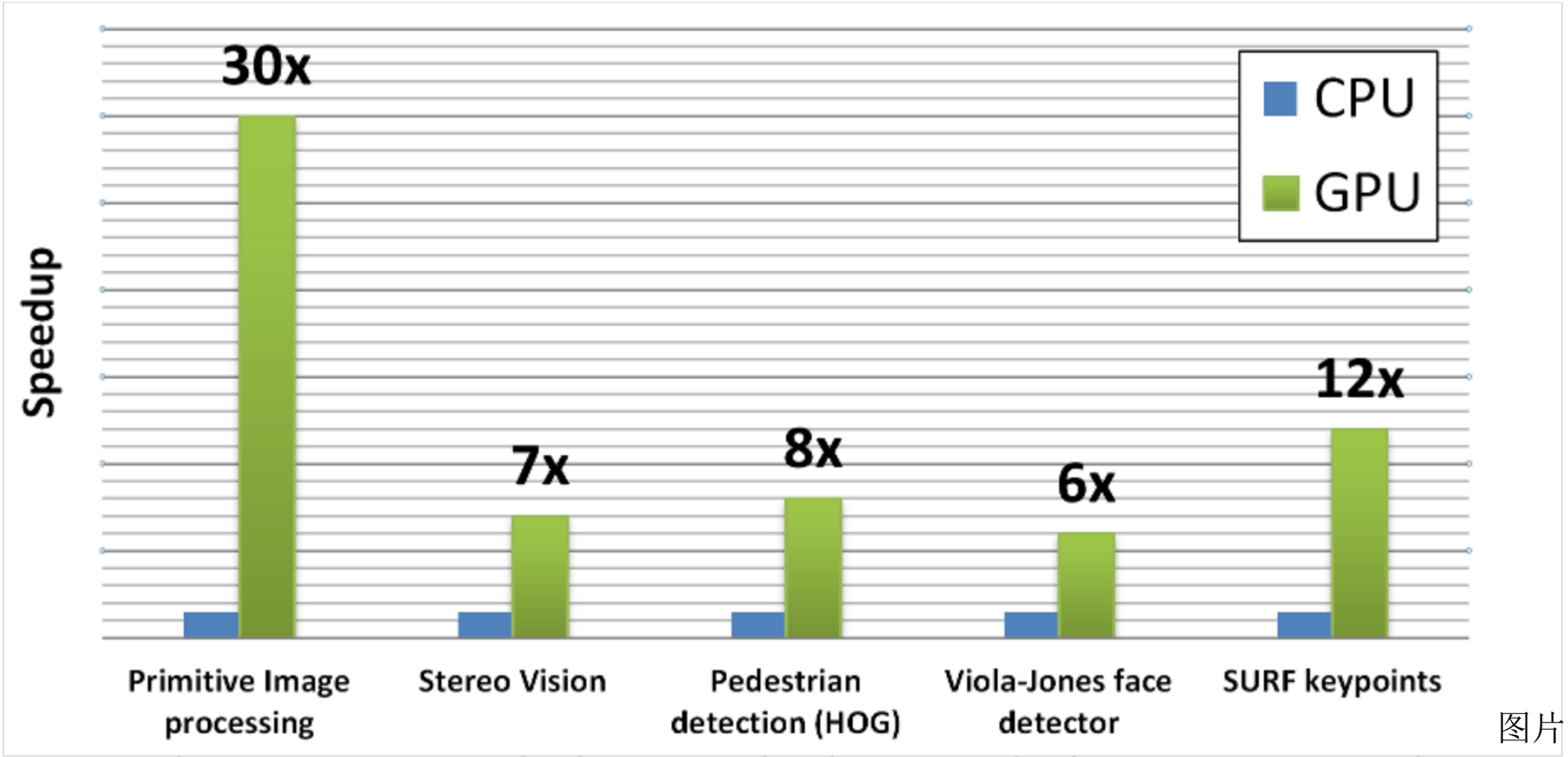
CUDA 加速效果

- 案例分析-矩阵乘法
  - 策略2：
    - 先创建 $n \times p \times m$ 个线程计算所有乘法
    - 再创建 $n \times p \times (m-1)$ 个线程计算所有加法
    - 更容易保持满载，但创建进程开销也更高



CUDA 加速效果

- OpenCV
  - 跨平台计算机视觉库

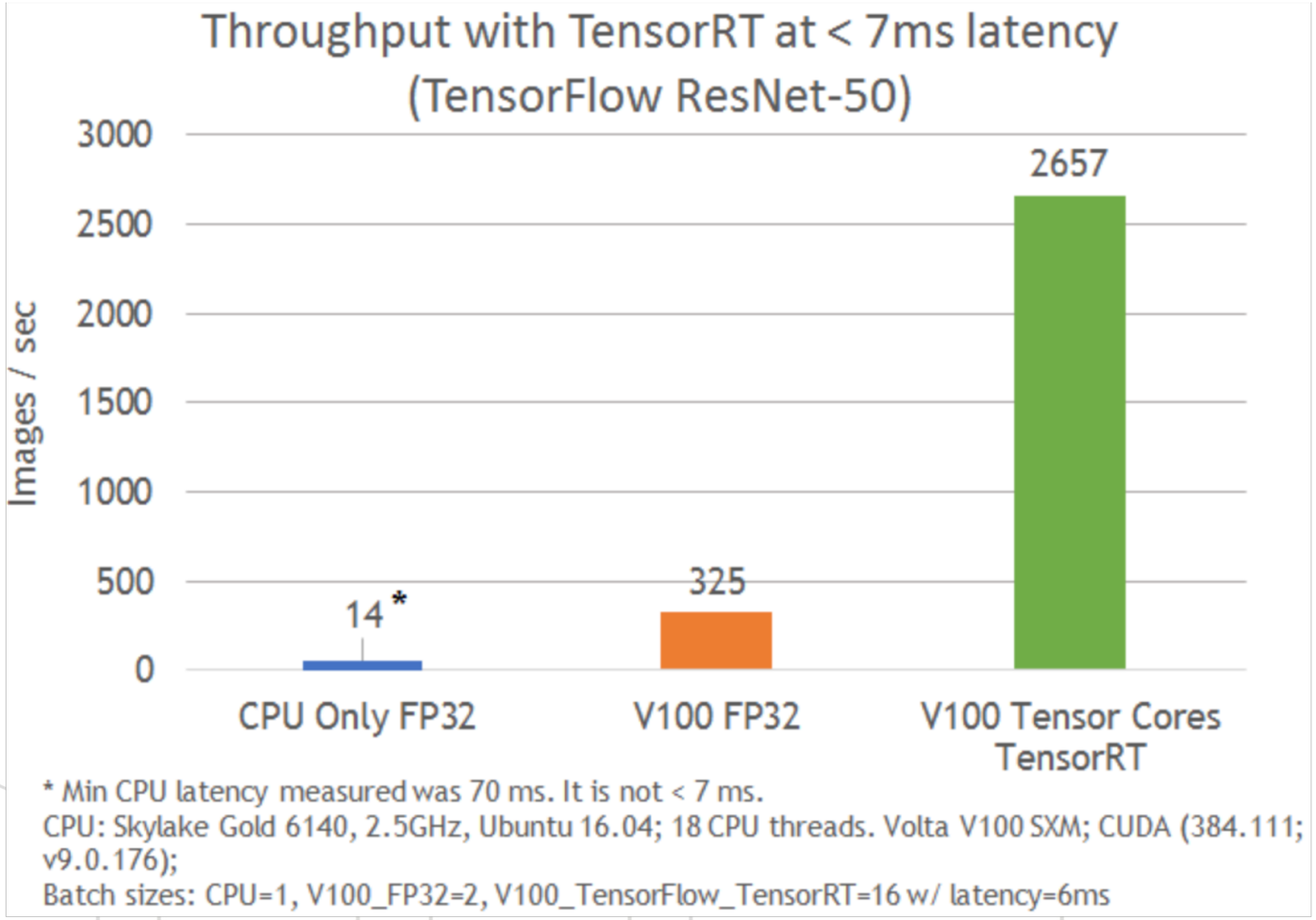


图片来自OpenCV.org

Tesla C2050 (448 cores) versus Core i5-760 2.8Ghz

CUDA 加速效果

- TensorFlow
  - 深度学习

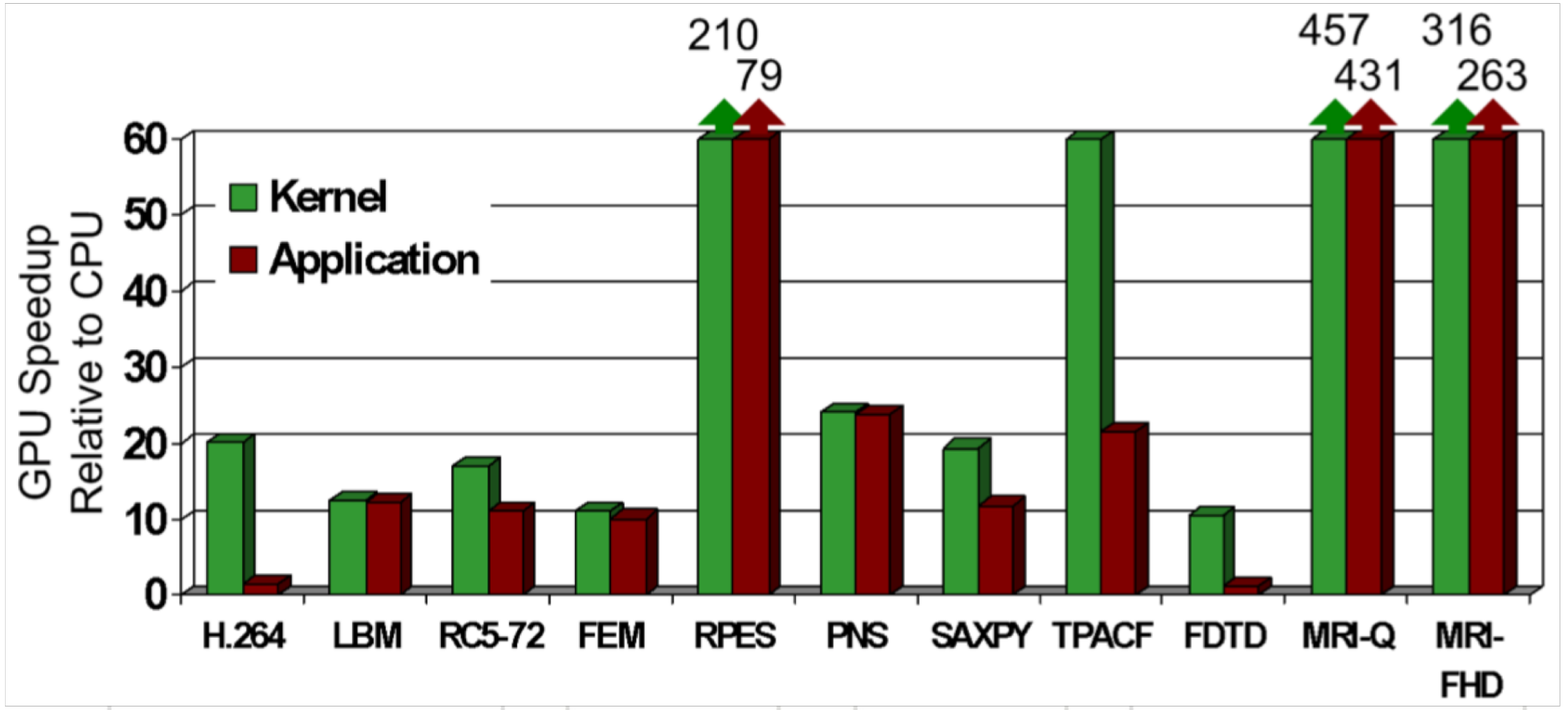


图片来自Laurence Moroney

CUDA 加速效果

UIUC ECE 498AL

– 课程项目

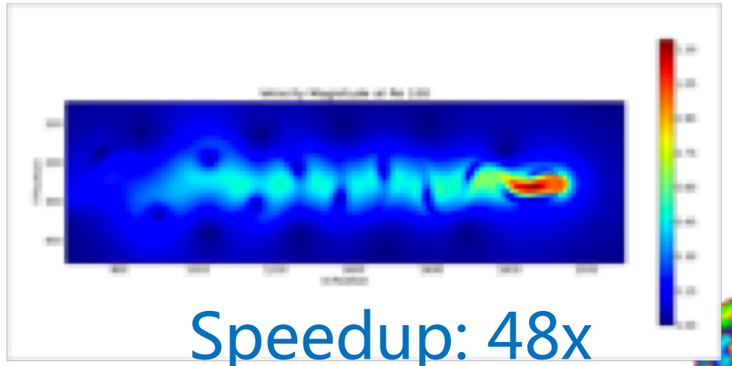


图片来自UIUC

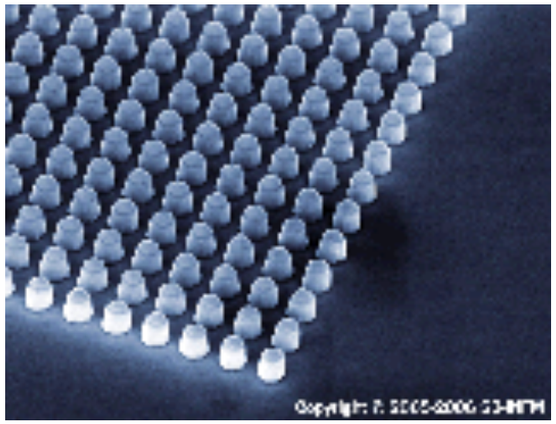
GeForce 8800 GTX（575核）vs 2.2GHz Opteron 248

CUDA 加速效果

CUDA Zone Showcase



Speedup: 48x



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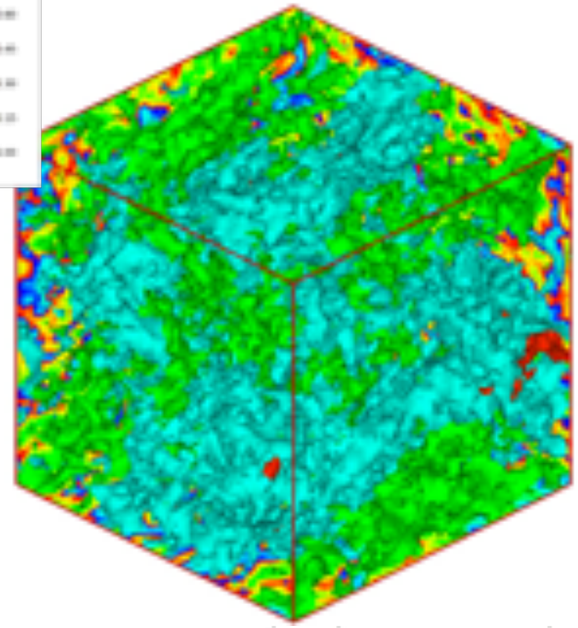
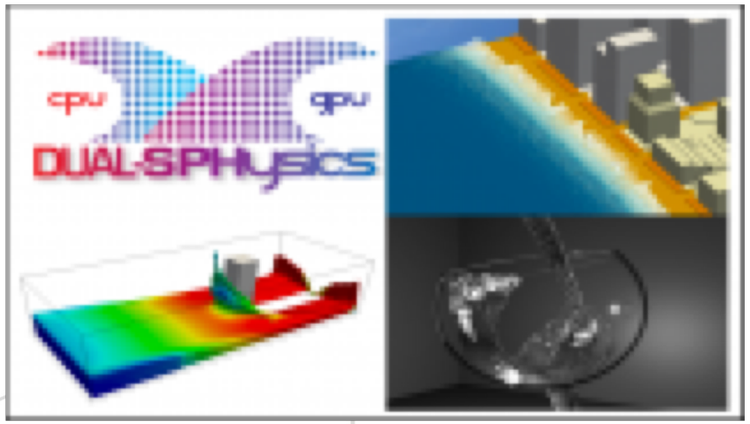


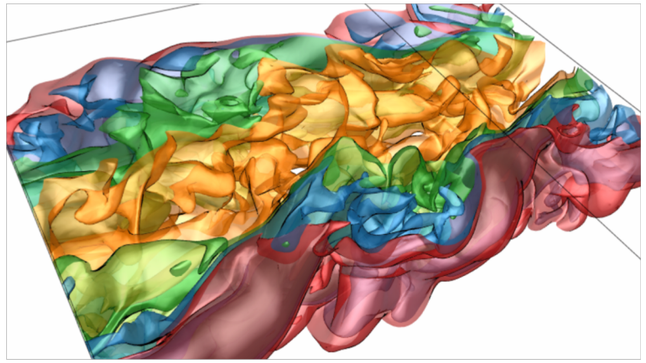
Speedup: 45x

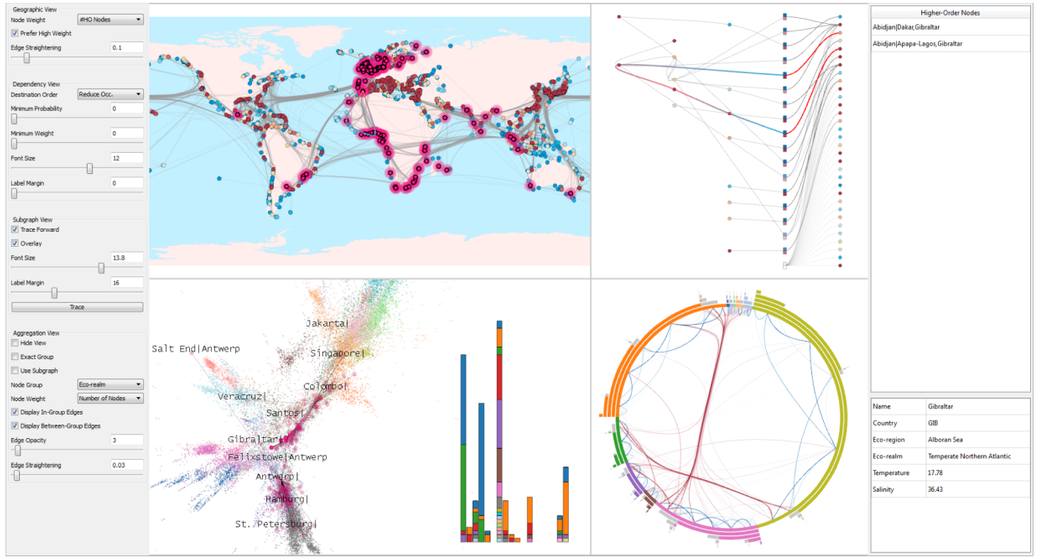


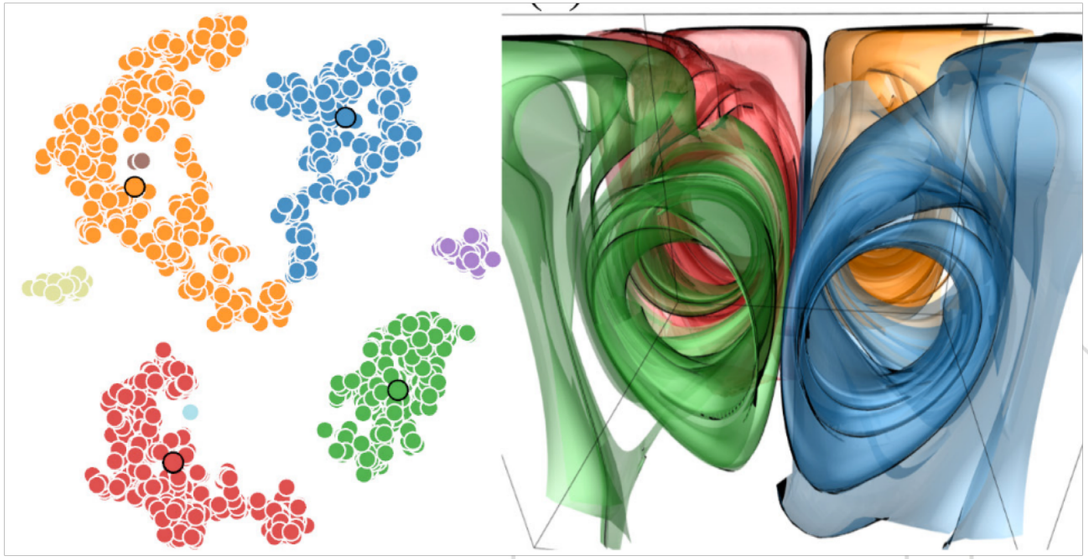
Speedup: 90x

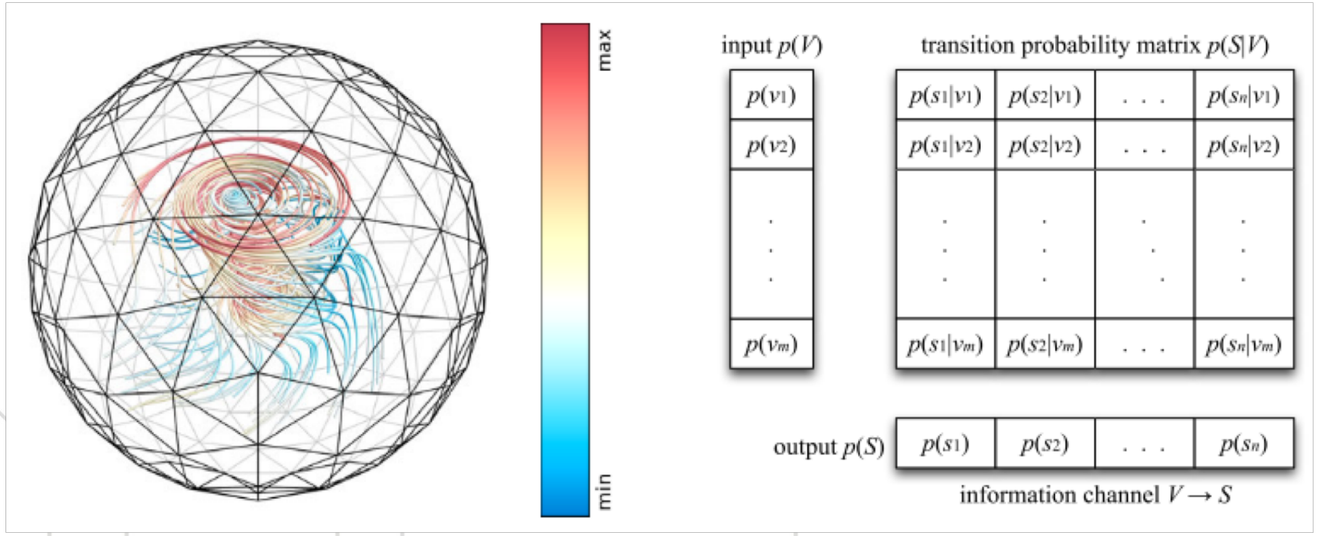
CUDA 加速效果

- 我的工作
  - 几乎都用到CUDA









课程概要

- 课程目标与评分标准
- Why CUDA?
- CUDA加速效果
- 安装与项目创建

安装

- 下载CUDA Toolkit
  - 下载地址： http://developer.nvidia.com/cuda-downloads
  - Toolkit
    - nvcc 编译器
    - visual profiler
    - visual studio integration (windows)
  - Samples
    - 基本功能：device query、band width query等
    - 线性系统：QR factorization, LU decomposition等
    - 图算法：最短路径、PageRank等
    - 模拟：粒子系统、ray tracing等
  - 显卡驱动

安装

– 参照说明文档

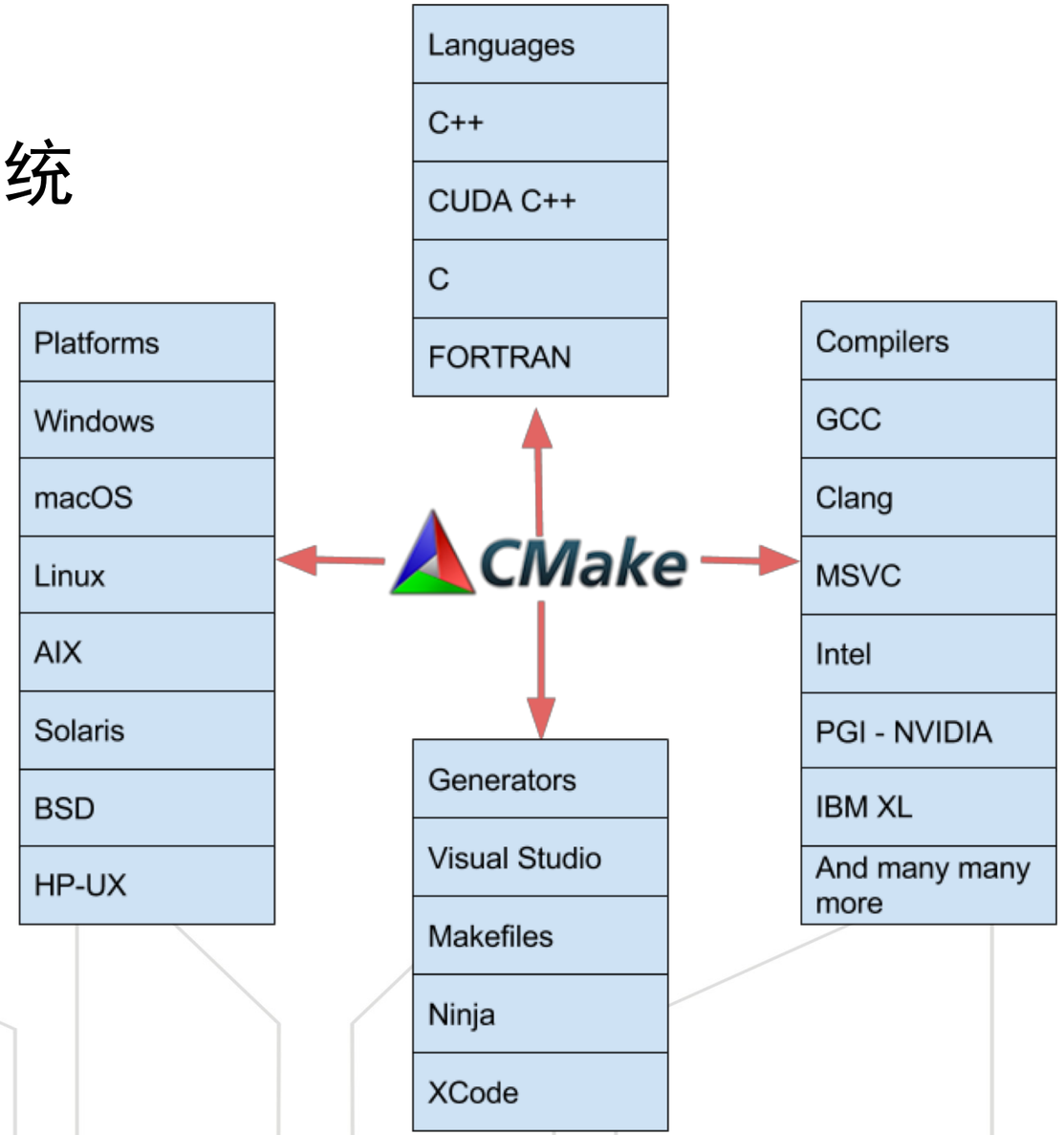
- https://docs.nvidia.com/cuda/cuda-installation-guide-microsoft-windows/index.html
- https://docs.nvidia.com/cuda/cuda-installation-guide-mac-os-x/index.html
- https://docs.nvidia.com/cuda/cuda-installation-guide-linux/index.html

安装成功后应该能通过deviceQuery查看支持CUDA的硬件状态

```
deviceQuery.exe Starting...

 CUDA Device Query (Runtime API) version (CUDART static linking)

Detected 1 CUDA Capable device(s)

Device 0: "GeForce GTX 680"
  CUDA Driver Version / Runtime Version          6.0 / 6.0
  CUDA Capability Major/Minor version number:    3.0
  Total amount of global memory:                 2048 MBytes (2147483648 bytes)
  ( 8) Multiprocessors, (192) CUDA Cores/MP:     1536 CUDA Cores
  GPU Clock rate:                                1059 MHz (1.06 GHz)
  Memory Clock rate:                             3004 Mhz
  Memory Bus Width:                              256-bit
  L2 Cache Size:                                 524288 bytes
  Maximum Texture Dimension Size (x,y,z)         1D=(65536), 2D=(65536, 65536), 3D=(4096, 4096, 4096)
  Maximum Layered 1D Texture Size, (num) layers  1D=(16384), 2048 layers
  Maximum Layered 2D Texture Size, (num) layers  2D=(16384, 16384), 2048 layers
  Total amount of constant memory:               65536 bytes
  Total amount of shared memory per block:       49152 bytes
  Total number of registers available per block: 65536
  Warp size:                                     32
  Maximum number of threads per multiprocessor:  2048
  Maximum number of threads per block:           1024
  Max dimension size of a thread block (x,y,z): (1024, 1024, 64)
  Max dimension size of a grid size    (x,y,z): (2147483647, 65535, 65535)
  Maximum memory pitch:                          2147483647 bytes
  Texture alignment:                             512 bytes
  Concurrent copy and kernel execution:          Yes with 1 copy engine(s)
  Run time limit on kernels:                     Yes
  Integrated GPU sharing Host Memory:            No
  Support host page-locked memory mapping:       Yes
  Alignment requirement for Surfaces:            Yes
  Device has ECC support:                        Disabled
  CUDA Device Driver Mode (TCC or WDDM):         WDDM (Windows Display Driver Model)
  Device supports Unified Addressing (UVA):      No
  Device PCI Bus ID / PCI location ID:           1 / 0
  Compute Mode:
     < Default (multiple host threads can use ::cudaSetDevice() with device simultaneously) >

deviceQuery, CUDA Driver = CUDART, CUDA Driver Version = 6.0, CUDA Runtime Version = 6.0, NumDevs = 1, Device0 = GeForce GTX 680
Result = PASS
```

创建项目

- CMake
  - 跨平台自动化建构系统



创建项目

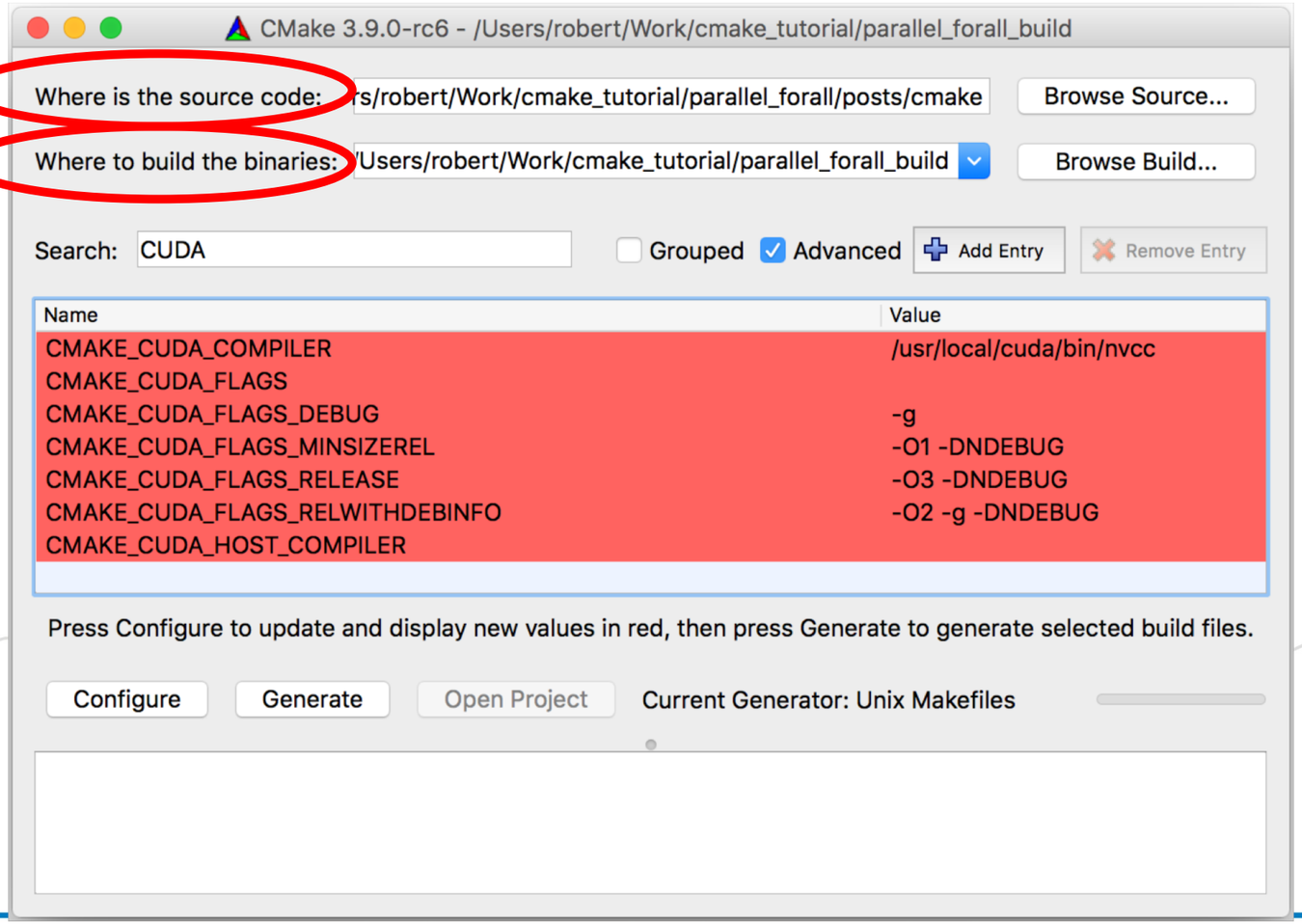
- CMake
  - 通过CMakeLists.txt 指明源文件、依赖关系、目标文件
    - 例子：

```
# 从helloworld.cu构建helloworld项目
# 检查cmake版本及自动寻找CUDA库路径
cmake_minimum_required(VERSION 2.8)
find_package(CUDA QUIET REQUIRED)

# 指明二进制可执行文件名称及源文件名称
cuda_add_executable(
    helloworld
    src/helloworld.cu)
```

创建项目

CMake

– 使用命令行或GUI创建项目文件



第一个程序

- 查询支持CUDA的硬件
  - 源码

```
int nDevices;
cudaGetDeviceCount(&nDevices);

for (int i = 0; i < nDevices; i++) {
    cudaDeviceProp prop;
    cudaGetDeviceProperties(&prop, i);
    printf(" Device Number: %d\n", i);
    printf(" Device name: %s\n", prop.name);
    printf(" Memory Clock Rate (KHz): %d\n", prop.memoryClockRate);
    printf(" Memory Bus Width (bits): %d\n", prop.memoryBusWidth);
    printf(" Peak Memory Bandwidth (GB/s): %f\n\n",
             2.0*prop.memoryClockRate*(prop.memoryBusWidth/8)/1.0e6);
}
```

  - 输出

```
Device Number: 0
Device name: Tesla C2050
Memory Clock Rate (KHz): 1500000
Memory Bus Width (bits): 384
Peak Memory Bandwidth (GB/s): 144.00
```

Questions?