并行与分布式计算

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School of Computer Science and Technology
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Bio

Education

- 1999/07, Computer Science, BS., Peking University
- 2001/12, Computer Engineering, MS., Northwestern University, USA
- 2005/06, Computer Engineering, Ph.D., Northwestern University, USA

Work Experience

- 2005/06 2005/11, Research Associate, Northwestern University, USA
- 2006/01 Present, Professor,
 University of Chinese Academy of Sciences

Bio

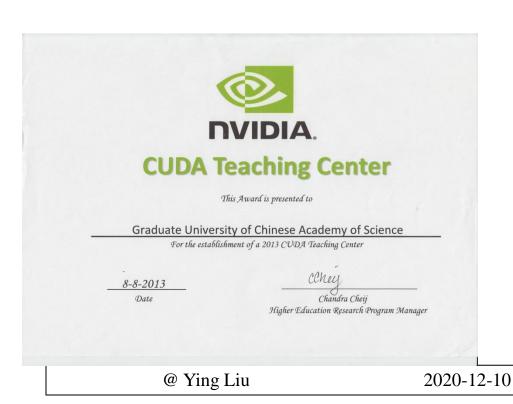
- Research interests
 - Data mining
 - High performance computing
 - Machine learning
 - Big data
- Contact: yingliu@ucas.ac.cn

University CUDA Courses (2010)

加州理工学院	美国伊利诺伊大学厄本那—香槟分校	斯图加特大学
斯坦福大学	美国北卡罗来纳州立大学	马里兰州大学
美国哈佛大学	美国东北大学	普渡大学
苏黎世理工学院	威斯康星大学	犹他大学
国佐治亚理工学院	美国俄勒冈州立大学	德国埃尔兰根大学
麻省理工学院	宾夕法尼亚大学	京都大学
印度国际信息技术学院	加拿大滑铁卢大学	瑞典兰德大学
印度理工学院(德里)	加拿大麦吉尔大学	东京大学
美国杜克大学	纽约州立大学	维也纳技术大学
法国国立信息与自动化研究院	华盛顿大学	威廉姆斯大学
澳大利亚西澳大学	弗吉尼亚大学	圣克拉拉大学
墨西哥蒙特雷理工大学	美国北卡罗来纳大学	美国格洛夫城市学院
约翰霍普金斯大学	美国南卡来罗纳大学	
肯特州立大学	美国爱荷华大学	

CUDA Teaching Center

- ▶ 率先在国内大学中开设《基于GPU并行计算》课程,被全球最大图形处理器公司NVIDIA授予2009年全球教授合作奖
- ▶ 2012年被授予全球CUDA教学中心称号





CUDA Teaching Center



Objectives

- Introduce a new emerging paradigm
- Introduce successful cases
- Provide students with knowledge and hands-on experience in developing multi-threaded code for GPUs using CUDA

Syllabus (Tentative)

- Introduction of CUDA
- CUDA Programming Model
- CUDA Memory
- CUDA Threads
- CUDA Performance Tune
- CUDA Advanced Topics

References

Websites

http://www.nvidia.com/

Documentation

 NVIDIA CUDA Programming Guide, NVIDIA. (https://docs.nvidia.com/cuda/cuda-c-programming-guide/)

Reference books

- CUDA范例精解--通用GPU编程(英文影印版), Jason Sanders, Edward Kandrot,清华大学出版社, 2010
- GPU高性能运算之CUDA, 张舒, 褚艳利, 中国水利水 电出版社, 2009

Outline

- GPU
- What is CUDA?
- Successful Cases
- Personal Supercomputer

TOP 10 Machines 11/2020

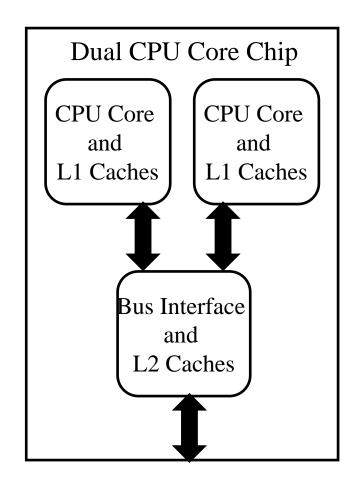
Rank	Name	Site	System	#core	R _{max} TF/s	Arch.	Country
1	Fugaku	RIKEN Center for Computational Science	Fugaku, A64FX 48C	7,630,848	442,010.0	MPP	Japan
2	Summit	DOE/SC/Oak Ridge National Laboratory	IBM Power System AC922, NVIDIA Volta GV100	2,414,592	148,600.0	cluster	USA
3	Sierra	DOE/NNSA/LLNL	IBM Power System S922LC, NVIDIA Volta GV100	1,572,480	94,640.0	cluster	USA
4	Sunway TaihuLight	National Supercomputing Center in Wuxi	Sunway SW26010 260C	10,649,600	93,014.6	MPP	China
5	Selene	NVIDIA Corporation	NVIDIA DGX A100, AMD EPYC 7742	555,520	63,460.0	cluster	United States

TOP 10 Machines 11/2020

Rank	Name	Site	System	#core	R _{max} TF/s	Arch.	Country
6	Tianhe-2A		TH-IVB-FEP cluster, Matrix-2000	4,981,760	61,444.5	cluster	China
7	JUWELS Booster Module	Forschungszentru m Juelich (FZJ)	Bull Sequana XH2000, AMD EPYC, NVIDIA A100	449,280	44,120.0	cluster	Germany
8	HPC5	Eni S.p.A.	Dell EMC PowerEdge C4140, Xeon Gold 6252 24C, NVIDIA Tesla V100		35,450.0	cluster	Italy
9	Frontera	Texas Advanced Computing Center/Univ. of Texas	Dell C6420, Xeon Platinum 8280 28C	448,448	23,516.4	cluster	USA
10	Dammam-7	Saudi Aramco	Cray CS-Storm, Xeon Gold 6248 20C, NVIDIA Tesla V100 SXM2	672,520	22,400.0	cluster	Saudi Arabia

Multi-Core

- A multi-core processor combines two or more independent cores into a single package composed of a single integrated circuit (IC), called a die.
- Each individual core is a CPU



Multi-Core

Pros

- Allow many users to connect to a site simultaneously and have independent threads
- Cores in a die share a single coherent cache
- Lower cost for higher performance
- Low power consumption

Cons

Design difficulty, 2-core => 4-core => 8 core =>......

Multi-Core

Hardware

Intel

- Celeron Dual Core, the first dual-core processor for the budget/entry-level market.
- Core Duo, a dual-core processor.
- Itanium 2, a dual-core processor.
- Pentium D, a dual-core processor.
- Nehalem, a quad-core processor, a 6-core processor, a 8-core processor.

AMD

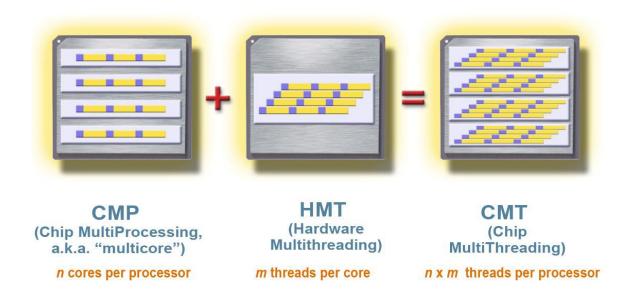
- Athlon 64, Athlon 64 FX and Athlon 64 X2 family, dual-core desktop processors.
- Opteron, dual- and quad-core server/workstation processors.
- Phenom, triple- and quad-core desktop processors.
- Turion 64 X2, dual-core laptop processors.

IBM

- POWER4, the world's first dual-core processor.
- POWER5, a dual-core processor.
- POWER6, a dual-core processor.
- PowerPC 970MP, a dual-core processor, in the Apple Power Mac G5.
- Sony/Toshiba/IBM Cell, 9 cores.

Programming on Multi-Core

- Multithreading
 - Parallel execution
 - Common data
 - Lock and barrier guarantees synchronization and data consistence



Programming on Multi-Core

Problem

- Heavy weight thread, 1000 cycles, launching, communication, synchronization, etc.
- Poor scalability on 8+ cores

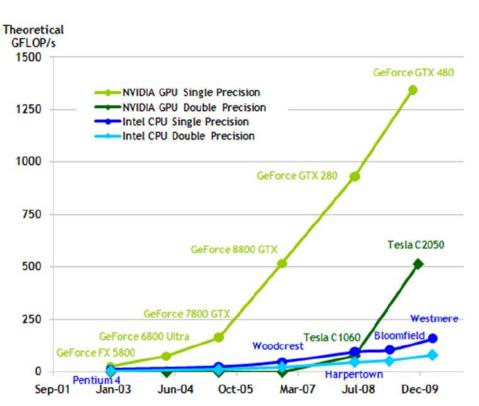
Good at

- Coarse grain
- Less communication
- Task parallelism

Parallel Computing with FPGA

- FPGA Vendors
 - Altera
 - Xilinx
- Embedded Reconfigurable System
 - Multi-channel data/signal processing in parallel
 - Standard/user defined interfaces with external system
 - Hard to co-program with HOST/CPU
 - Multi-blocks and multi-chips in parallel
 - Difficult to develop and debug

GPU (Graphic Processing Unit)





GPU



- Architecture difference between GPU and CPU
 - More transistors for data processing
 - Many-core (hundreds of cores)

Historic GPGPU Movement

- General Purpose computation using GPU in applications other than 3D graphics
 - GPU accelerates critical path of application
- Data parallel algorithms leverage GPU attributes
 - Large data arrays, streaming throughput
 - Fine-grain SIMD parallelism
 - Low-latency floating point (FP) computation



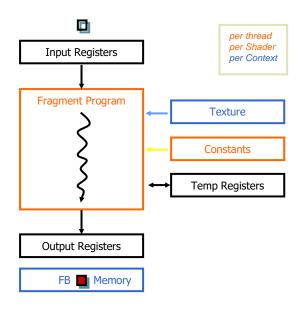
- Applications see http://GPGPU.org
 - Game effects (FX) physics, image processing
 - Physical modeling, computational engineering, matrix algebra, convolution, correlation, sorting

What is GPU Good at?

- Advantages of GPU
 - Low cost (hundreds of US dollars)
 - Many threads (hundreds or thousands of threads)
- Good at data-parallel processing
 - The same computation executed on many data elements in parallel – low control flow overhead with high floating point arithmetic intensity
 - Many calculations per memory access

Historic GPGPU Constraints

- Dealing with graphicsAPI
 - Working with the corner cases of the graphics API
- Addressing modes
 - Limited texture size/dimension
- Communication limited
 - No interaction between pixels

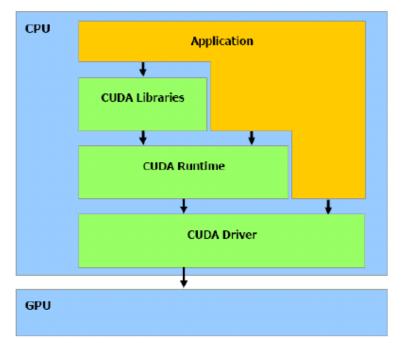


Outline

- GPU
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- Successful Cases
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CUDA (Compute Unified Device Architecture)

- Write programs for GPU on C language with minimum extensions
- Ease of programming
- Single Program Multiple Data (SPMD)
- No need of graphics APIs



Software Stack

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CUDA API Highlights: Easy and Lightweight

- The API is an extension to the ANSI C programming language
 - Low learning curve

- The hardware is designed to enable lightweight runtime and driver
 - High performance

TOP 500 Machines 11/2020

Global

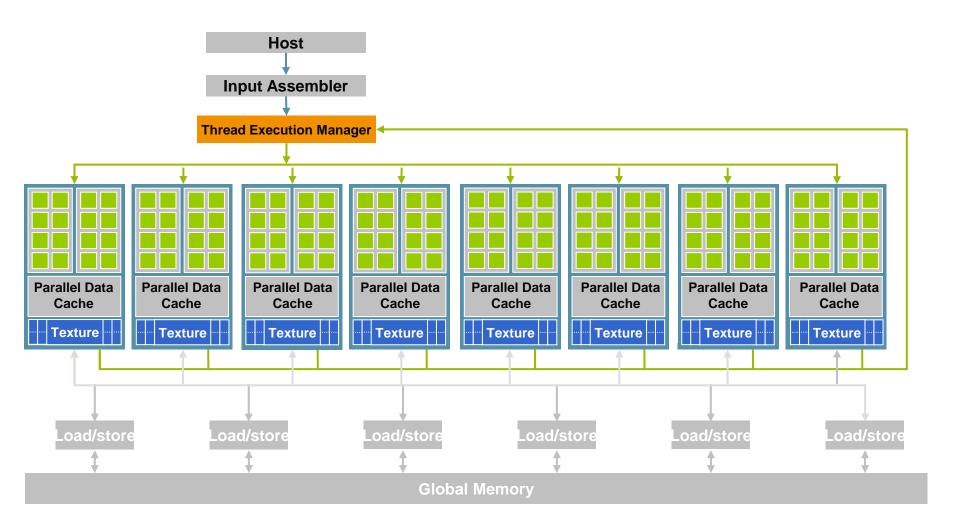
- 6/10 Nvidia CUDA GPUs as co-processors
- 140/500 Nvidia CUDA GPUs as co-processors
- 9/500 Intel Xeon Phi as co-processors

G80 – Graphics Mode



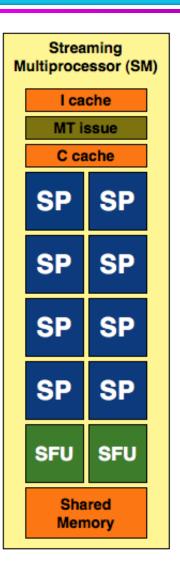
Block Diagram of the GeForce 8800

G80 CUDA Mode

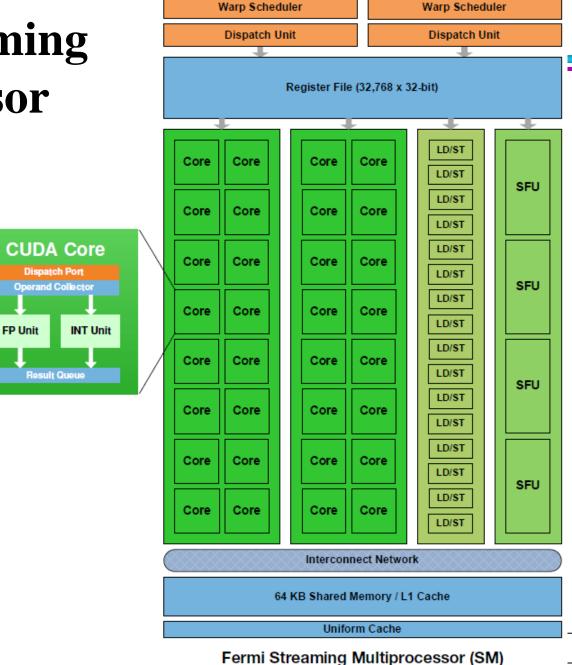


Streaming Multiprocessor (SM)

- An array of SPs
 - 8 streaming processors
 - 2 Special Function Units (SFU)
 - Transcendental operations (e.g. sin, cos) and interpolation
 - A 16KB read/write shared memory
 - Not a cache, but a softwaremanaged data store
 - Multithreading issuing unit
 - Dispatch instructions
 - Instruction cache
 - Constant cache



Fermi Streaming Multiprocessor (SM)



Instruction Cache

CUDA Device

- A compute device
 - Is a coprocessor to the CPU or host
 - Has its own DRAM (device memory)
 - Runs many threads in parallel
 - Is typically a GPU but can also be another type of parallel processing device
- Kernel Data-parallel portions of an application which run on many threads

GPU+CUDA

- CUDA integrated CPU+GPU application C program
 - Serial or modestly parallel C code executes on CPU
 - Highly parallel SPMD kernel C code executes on GPU

CPU Serial Code Grid 0 GPU Parallel Kernel KernelA<<< nBlk, nTid >>>(args); **CPU Serial Code** Grid 1 GPU Parallel Kernel KernelB<<< nBlk, nTid >>>(args); 2020-12-10 @ Ying Liu

Block IDs and Thread IDs

Each thread uses IDs to decide what data to work on

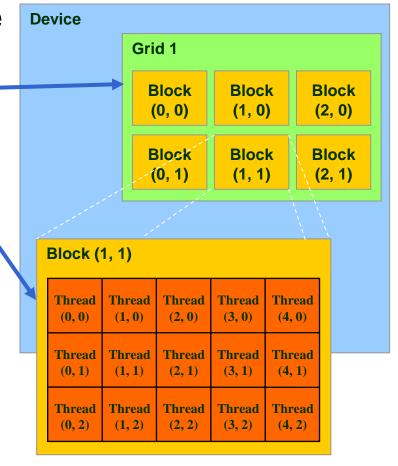
Block ID: 1D or 2D

Thread ID: 1D, 2D, or 3D

 Simplify memory addressing when processing multidimensional data

- Image processing
- Solving PDEs on volumes

• ...



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支持CUDA的NVIDIA硬件

GeForce[®] 娱乐

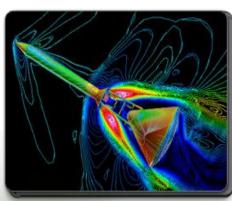
Quadro® 设计和创作

Tesla™ 高性能计算

Tegra 嵌入式系统









GPU

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Configuration

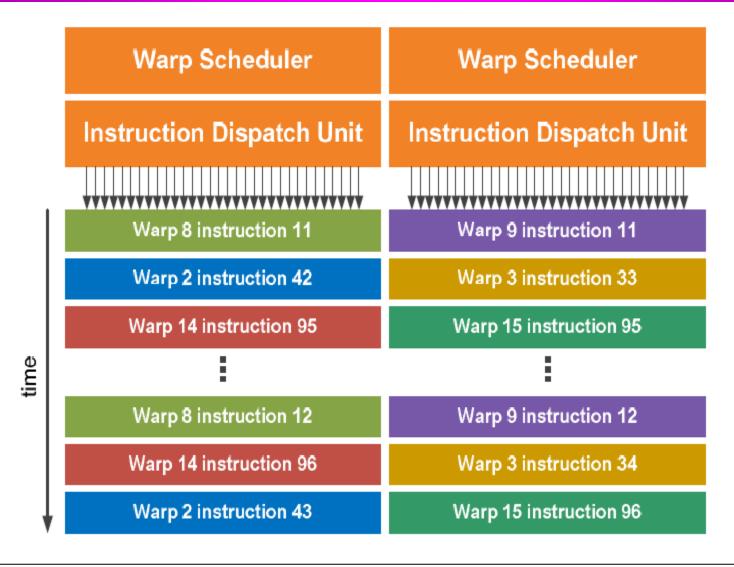
	GeForce 8800 GTX	Tesla C1060 (GTX280)
# stream processor	128	240
# stream multiprocessor	16	30
# registers per SM	8192 (32KB)	16384(64KB)
# threads per block	Up to 512	Up to 512
# threads per SM	Up to 768	Up to 768
# blocks per SM	Up to 8	Up to 8
# blocks per grid	Up to 65535 each dim	Up to 65535 each dim
global memory	768MB, 1.8GHz, 384-bit	4GB, 1.6GHz, 512-bit
constant memory	64KB	64KB
shared memory per SM	16KB	32KB
clock	1.35GHz	1.296GHz
peak	346.5 GFlops/s	936 GFlops/s
memory bandwidth	86.4 GB/s	102 GB/s

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New Features in Fermi

- 512 SPs in total
- 32 SPs per SM, 4x over GT200
- 4 SFUs per SM
- 64 KB on-chip memory per SM
 - Can be configured as 48 KB of Shared memory with 16 KB of L1 cache or as 16 KB of Shared memory with 48 KB of L1 cache
- Dual Warp Scheduler simultaneously schedules and dispatches instructions from two independent warps

Fermi Dual Warp Scheduler

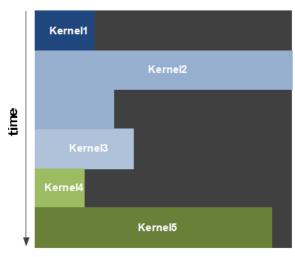


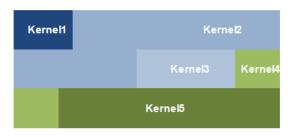
@ Ying Liu

2020-12-10

New Features in Fermi

- Support full C++
- Up to 20x faster atomic memory operations
- Concurrent kernel execution
 - Different kernels of the same application context can execute on the GPU at the same time





Serial Kernel Execution

Concurrent Kernel Execution

Configuration

GPU	G80	GT200	Fermi
Transistors	681 million	1.4 billion	3.0 billion
CUDA Cores	128	240	512
Double Precision Floating	None	30 FMA ops / clock	256 FMA ops /clock
Point Capability			
Single Precision Floating	128 MAD	240 MAD ops /	512 FMA ops /clock
Point Capability	ops/clock	clock	
Special Function Units	2	2	4
(SFUs) / SM			
Warp schedulers (per SM)	1	1	2
Shared Memory (per SM)	16 KB	16 KB	Configurable 48 KB or
			16 KB
L1 Cache (per SM)	None	None	Configurable 16 KB or
			48 KB
L2 Cache	None	None	768 KB
ECC Memory Support	No	No	Yes
Concurrent Kernels	No	No	Up to 16
Load/Store Address Width	32-bit	32-bit	64-bit

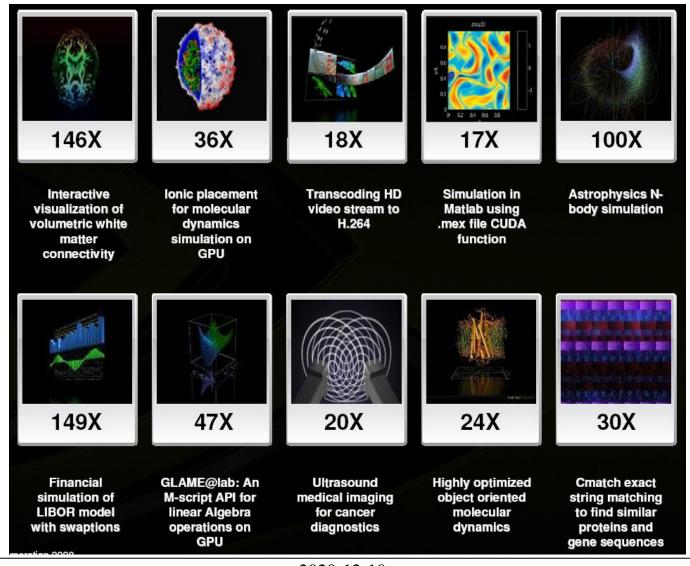
Free Downloadable CUDA Software

- https://developer.nvidia.com/
 - CUDA driver
 - CUDA toolkit
 - CUDA SDK
 - CUDA Visual Profiler

Outline

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Successful Applications

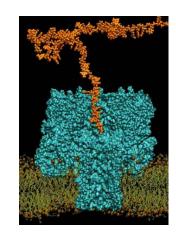


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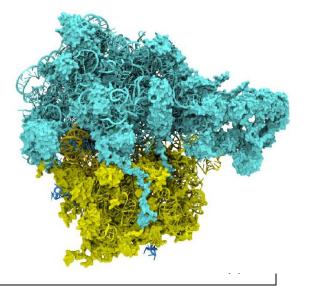
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VMD

Calculation / Algorithm	Algorithm class	Speedup vs. Intel QX6700 CPU core
Fluorescence microphotolysis	Iterative matrix / stencil	12x
Pairlist calculation	Particle pair distance test	10-11x
Pairlist update	Particle pair distance test	5-15x
Molecular dynamics non- bonded force calculation	N-body cutoff force calculations	10x 20x (w/ pairlist)
Cutoff electron density sum	Particle-grid w/ cutoff	15-23x
Cutoff potential summation	Particle-grid w/ cutoff	12-21x
Direct Coulomb summation	Particle-grid	44x

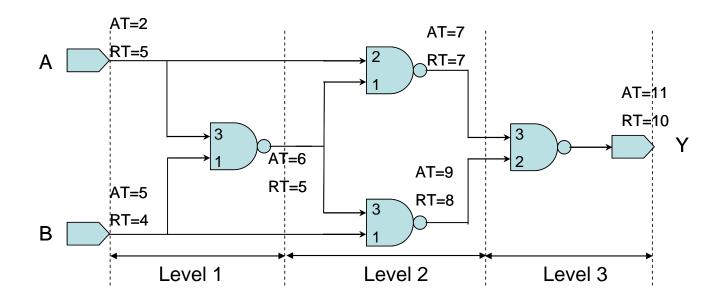


Theoretical and Computational Biophysics Group, UIUC http://www.ks.uiuc.edu/Research/gpu/



EDA

- Graph theory algorithms (20-50X)
 - breadth first traversal
 - single source shortest path
 - all pair shortest path
 - maximum flow, Push re-label



Numerical Weather Prediction (NWP)

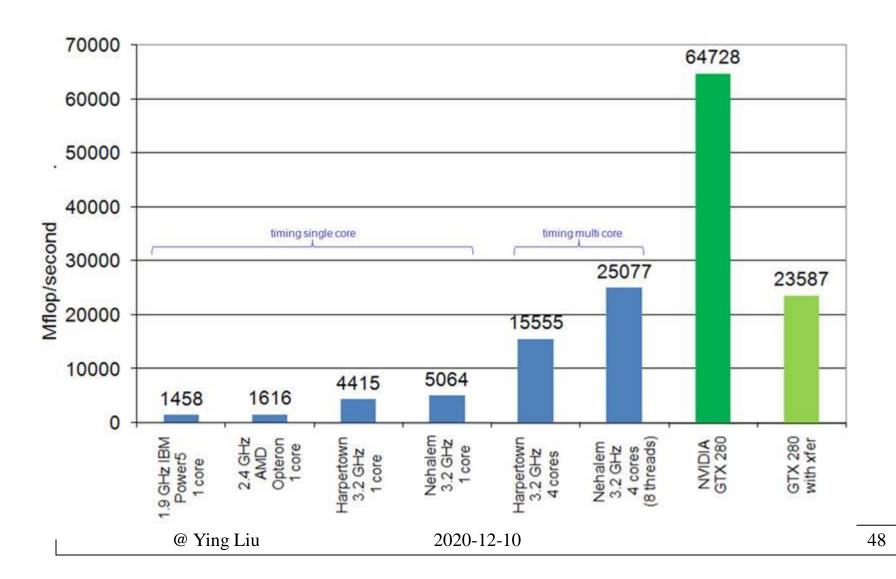
- Weather Research and Forecast Model (WRF)
- WRF Single Moment 5-tracer (WSM5)
 - 0.4% of the WRF code but consumes 25% total run time

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CUDA Implementation

- Geographical region partitioned in a 2D grid parallel to the ground
- Multiple levels along vertical height in the atmosphere for each grid
- 2400 floating point multiply-equivalent operation per cell per invocation
- Use -use_fast_math option to nvcc compiler
 - Square root, log, exponent to be computed by SFUs on the GPU
- Eliminate temporary arrays that store results between successive loops over k, the vertical dimension of WRF domain

Evaluation

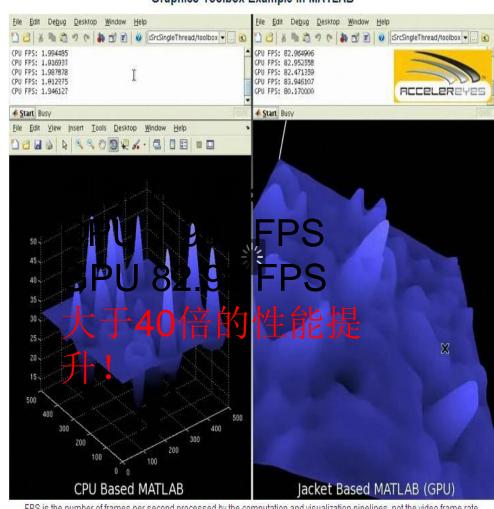


GPU 加速MATLAB — Jacket 插件

- MATLAB被广泛地应用于科学计算、控制系统、信息处理、医疗成像仿真等领域的分析、仿真和设计工作
- Jacket是由AccelerEyes公司 开发的一个强大的基于 CUDA的MATLAB 插件
- 性能提高 40 倍以上
- 支持 Win 32/64, Linux 32/64, Mac 32

http://www.accelereyes.com

Graphics Toolbox Example in MATLAB



FPS is the number of frames per second processed by the computation and visualization pipelines, not the video frame rate.

(Last Updated: 07 September 2008)

GPU 加速矢量信号图像处理库 VSIPL 20 至 350 倍

- GPU VSIPL 实现了 VISPL Core Lite Profile
- 用CUDA 2.3 和 Visual Studio 2005 实现
- 在 GeForce 8800GTX 上 20 至350 倍的加速
- 支持 Windows XP/Vista, Linux

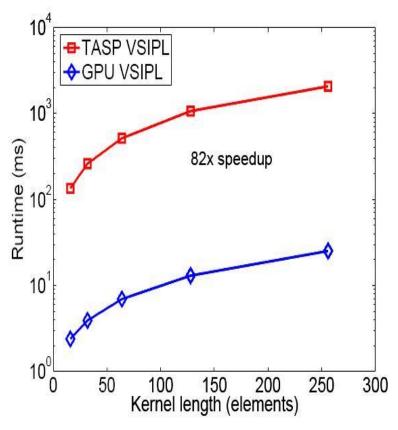
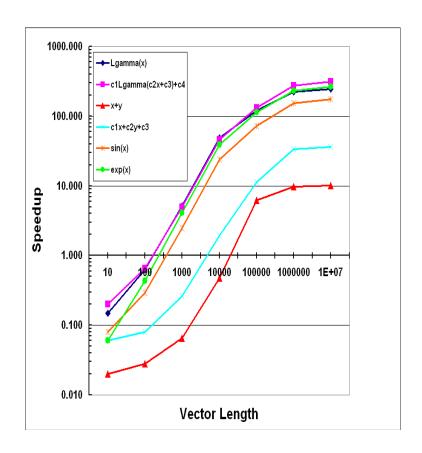


Figure 1: Time-domain FIR filtering runtime.

http://gpu-vsipl.gtri.gatech.edu/

GPU 加速数学库 — Tech-X 的 GPULib

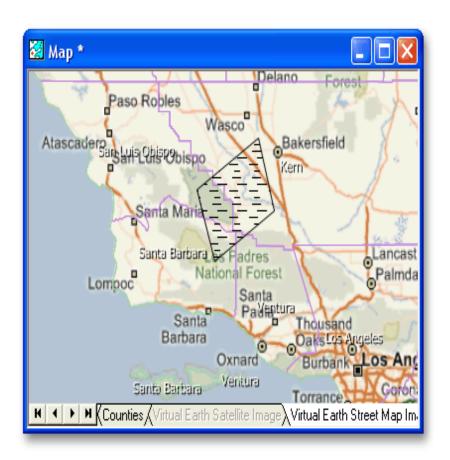
- GPULib 提供了基于GPU的 数学库
- 不需要GPU编程的知识
- 30 倍的加速



http://www.txcorp.com/products/GPULib/

GPU 加速 GIS 应用 — Manifold 8

- Manifold 8 是第一个支持 GPU的地理信息系统
- 利用GPU,GIS任务和分析比以前快几百倍



http://www.manifold.net/index.shtml

GPU加速分子建模应用软件 — OpenMM

- OpenMM 在 GPU 上加速 GROMACS
- 高达 10 至 1000 的加速
- 支持 MacOS, Windows, Linux

Molecule	# atoms	ns/day	speedup*	GFLOPS (GPU)	GFLOPS (x86)
fip35	544	576	128	311	657
villin	582	529	136	328	692
lambda	1254	202	255	547	1153
a- spectrin	5078	17	735	805	1702

(*comparing a GTX280 to a single core of a 3GHz core 2 duo using the AMBER code)

https://simtk.org/project/xml/downloads.xml?group_id=161

GPU加速分子建模应用软件 – 100x 伊利诺依大学NAMD / VMD

- 117 billions evals/sec
- 863 GFLOPS
- 131 倍的加速 (相对于 CPU核)





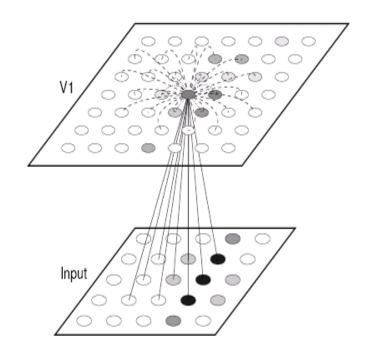
Quad-core Intel QX6700 3 块 NVIDIA GeForce 8800GTX

人类大脑模拟软件 — RF-LISSOM

■ 参见:

http://homepages.inf.ed.ac.uk/jbednar/rflissom_small.html

■ GT200 加速 5x 以上

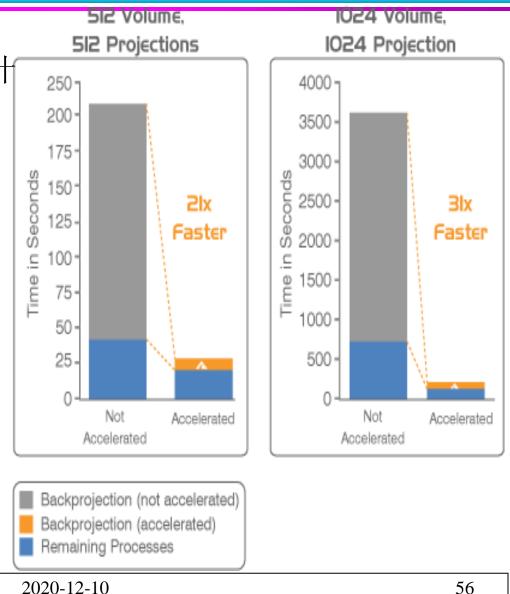


GPU 加速CT机的成像 — AxRecon

强大的性能,不再需要计 算集群

节省电力

■ 无损图像质量

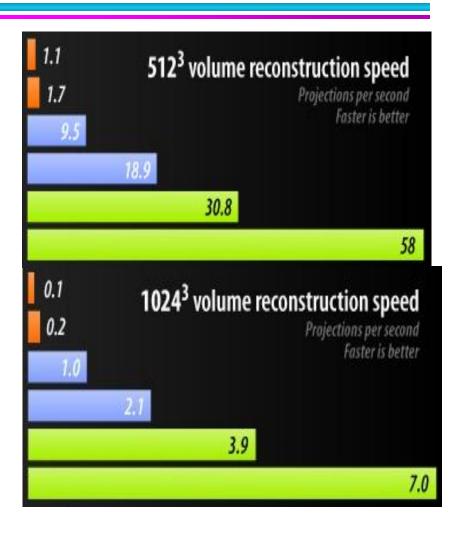


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GPU 加速CT机的成像 — SnapCT

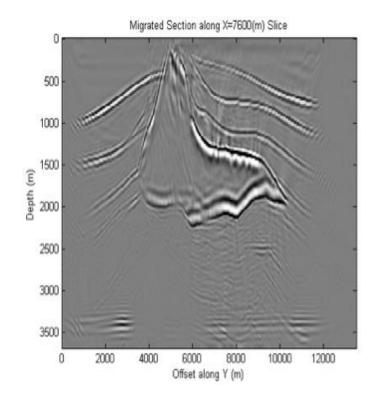
■ 性能提高 20~50 倍



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GPU加速 RTM 和 KTM

- 基尔霍夫叠前时间偏移(KTM)和反向时间偏移(RTM)是石油天然气行业常 用的数据处理手段
- Acceleware的GPU 方案节省 70%的电力
- 性能提高 20倍以上
- 参见:
 http://www.acceleware.com/d
 efault/index.cfm/solutions/sei
 smic-solutions/



GPU加速叠前深度偏移的3D 地震成像

- SeismicCity 现在在利用 NVIDIA Tesla S1070 进行叠 前深度偏移的成像处理
- 性能提高 60倍以上
- 参见:
 http://www.seismiccity.com/in
 dex.html



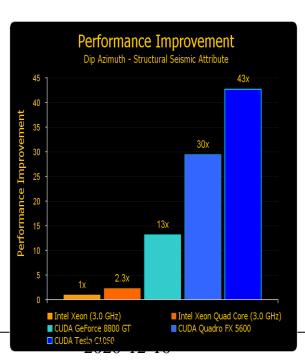
GPU加速频谱分析和反演

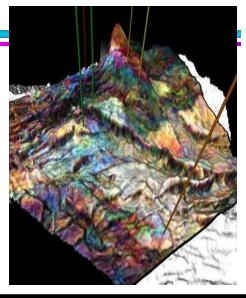
- OpenGeoSolutions公司专门使用一项叫做"光谱分析"的技术来提供地质信息,这些信息超越了传统的地震资料分辨率以及检测方式,在处理巨大的地区数据集时提高了数据质量。更重要的是,这种技术在逆向转换数据时还能够将其转换为真实的地质构造。
- OpenGeoSolutions利用NVIDIA Tesla C1060 进行光谱分析和反演,性能提高了数十倍。
- http://www.opengeosolutions.com/

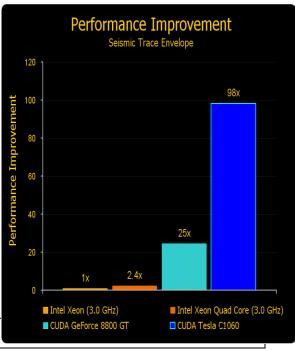
GPU加速地震属性的计算

- ffA是英国一家专门从事 3D地震成像处理技术的 公司。
- SEA 3D & SVI Pro 是
 ffA 公司3D地震成像分析和可视化的软件。
- 利用NVIDIA GPU性能 提高了10~100 倍。
- 参见:

http://www.ffa.co.uk/index.html





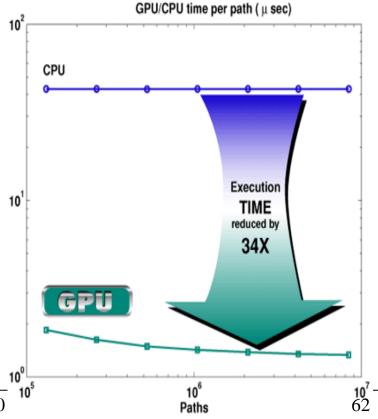


GPU加速定价模型

■ SciFinance 是专门从事建 造衍生定价和风险模型的 公司

■ 利用CUDA技术, Monte Carlo定价模型性能提高 30~100 倍

Serial	OpenMP (quad-core PC)	Single GPU	Dual GPU
43.3	11.0 sec	1.27	0.77
sec		sec	sec
	(x 3.94)	(x 34)	(x 56)

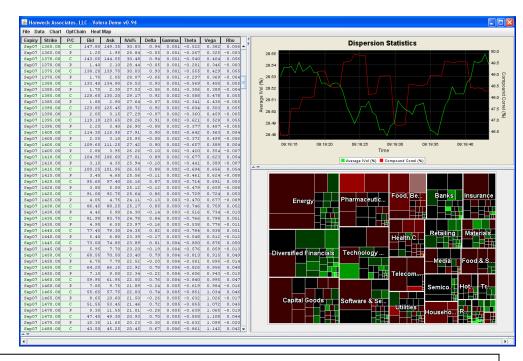


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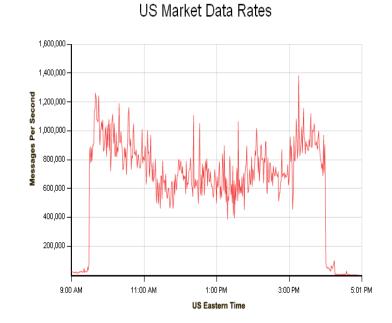
GPU加速期权定价

- VOLERA、实时期权隐含波动引擎
- 单精度的准确结果
- 在不到1秒钟的时间内,评估所有美国上市的股票期权
- 参见: <u>www.hanweckassoc.com</u>



GPU加速风险分析

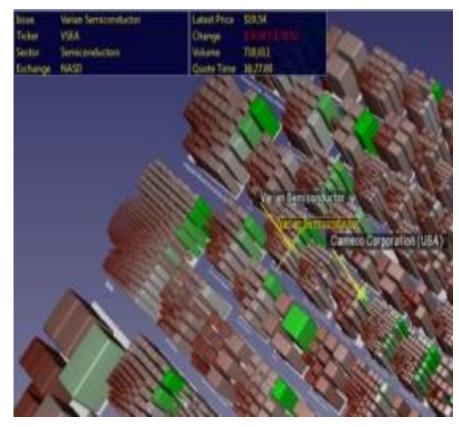
- Exegy 是专门为实时数据 处理提供硬件加速的公司
- 利用 Nvidia GPU, 性能提 高 180 倍
- 参见: http://www.exegy.com/PD Fs/WHT-0001-A_final.pdf



GPU加速市场数据三维可视化

- AQUMIN 是一家金融工具提 供商
- Aqumin 的 AlphaVision 把 金融数字转换为三维模式, 以更加直观的方式显示
- 参见: https://www.aqumin.com/H

ome/tabid/36/Default.aspx



人工智能

Images



image search

Audio



speech recognition

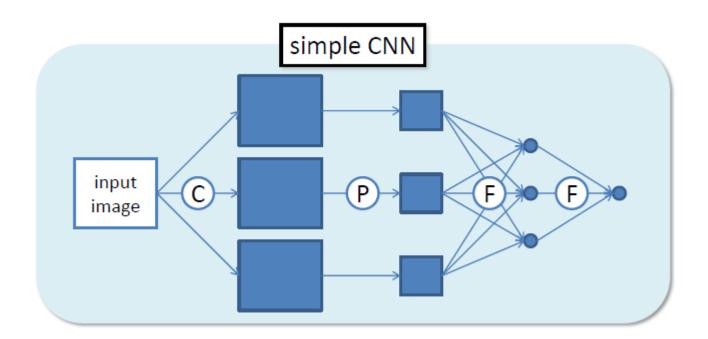
Text



Web search

Deep Neural Network

- Convolutional Neural Network (CNN) comprising
 - Convolutional layer(s) -> local feature extraction
 - Pooling layer(s) -> dimensionality reduction
 - Fully-connected layer(s) -> classification/regression



visual feature

automatically

extracted

Image Classification by Baidu

- Trained on millions+ images, up to 1.2 billions parameters
- Real-time prediction/classification is required

Infrastructure

Heterogeneous computing (CPU + GPU) by Baidu







Data center containers

- Faster deployment

Self-design switches

Much lower cost





Results by Baidu

- Datasets
 - Image recognition: 100 millions
 - Speech: 10 billions
 - Projected training data to grow 10x each year
- Training time: weeks to months
- Big improvement on speech & image recognition
 - Speech: error rate reduced by 25%
 - Face: LFW benchmark, 94% correct

Outline

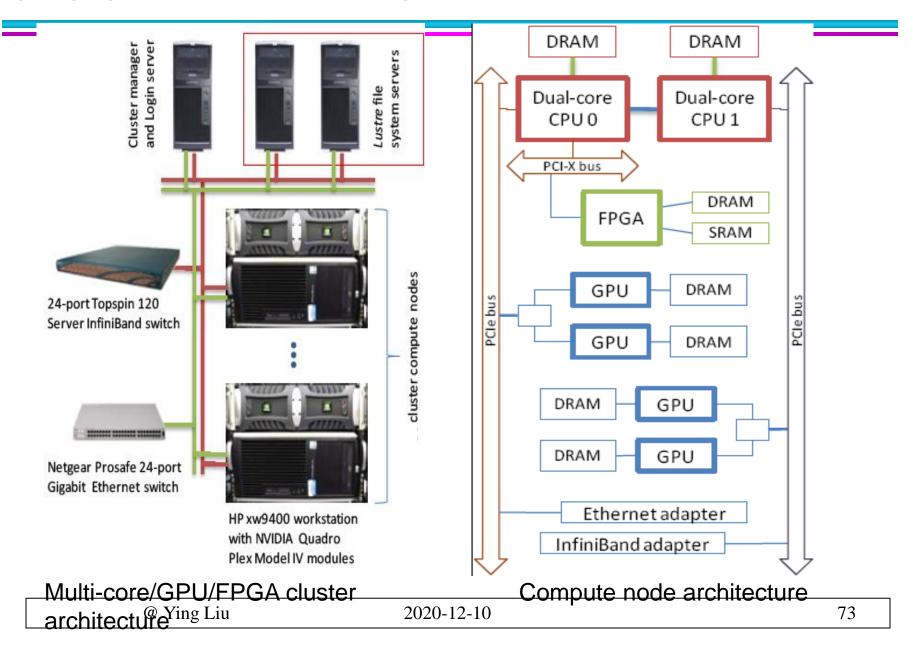
- GPU
- What is CUDA?
- Successful Cases
- Personal Supercomputer

Accelerator Cluster

- Combining GPU and FPGA
- 32 compute nodes:
 - 2 dual-core 2.4 GHz AMD Opterons
 - 8 GB host memory
 - 1 NVIDIA Tesla S1070 containing 4 GT200 GPUs, each with 4 GB memory
 - PCI-E GEN 2 cable
 - Nallatech H101-PCIX FPGA accelerator, 16 MB SRAM, 512
 MB SDRAM
- 2GB/sec InfiniBand connection
- Red Hat Enterprise Linux 5
- GNU C/Fortran and Intel C/Fortran compilers
- CUDA 2.0

http://www.ncsa.uiuc.edu/Projects/GPUcluster

UIUC Accelerator Cluster



多GPU集群的网络连接

- 服务器节点之间的连接:InfiniBand
 - 目前全球带宽最高的高速网络互联技术
 - 专门针对服务器端的连接而设计
 - 高扩展性: 在每个子网内支持上万个节点
 - 高吞吐量: 2008年已达到40Gb/sec
 - 低延迟: 1 微秒,以太网的1/10
- 集群子系统之间的连接: 千兆以太网

NVIDIA 打造性能强大的个人超级计算机



AMAX(美国)、Armari(英国) 、华硕(全球)、Azken Muga(西班 牙)、Boxx(美国)、CAD2(英国)、CADnetwork(德国)、Carri(法国)、Colfax(美国)、 Comptronic(德国)、Concordia(意 大利)、Connoisseur(印度)、戴尔 (全球)、Dospara (日本)、E-Quattro(意大利)、Founder(中国),Inspur (中国),JRTI(美国)、 联想(全球)、Littlebit(瑞士)、 Meijin (俄罗斯)、Microway (美国)、Sprinx(捷克)、Sysgen(德国)、Transtec(德国)、Tycrid (美 国)、Unitcom(日本)、Ustar(乌 克兰)、Viglen(英国)、Western Scientific (美国)

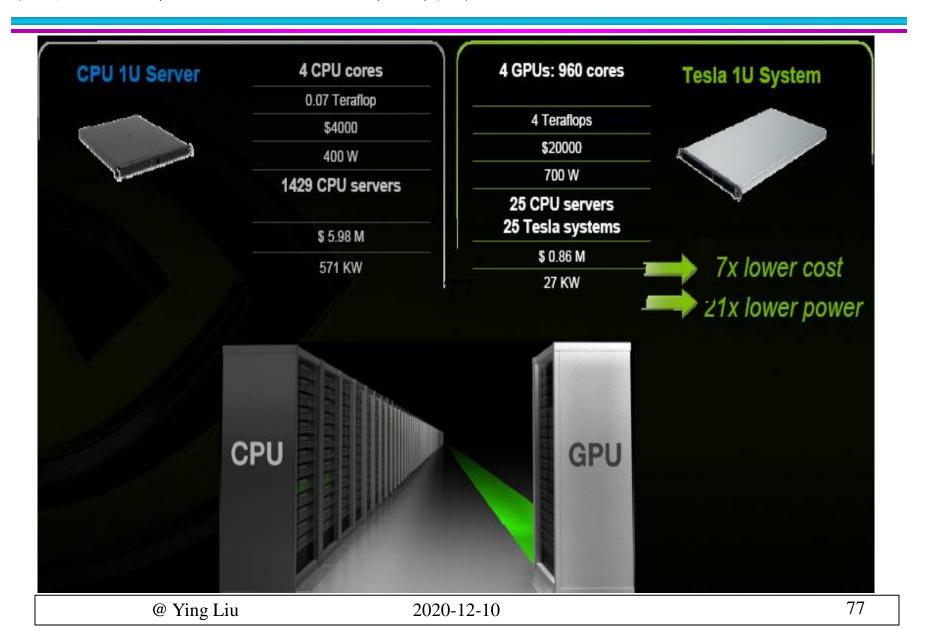
"Democratization" of Power

Name	Year	# Processors	Tflops/\$1 million
ILLIAC IV	1976	64	0.0000048
CRAY Y-MP	1988	8 vector processors	0.000115
ASCI RED	1997	4510	0.01818182
EARTH SIMULATOR	2002	5120	0.0175
BLUE GENE/L	2004	65536	2.8
PLAYSTATION 3 CLUSTER	2007	8 PlayStation 3s	375
ROADRUNNER	2008	19440	8.3
NVIDIA TESLA	2008	960 cores	439.1

Personal Supercomputer!

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搭建一个100 TF的数据中心



A Great Opportunity for Many

- GPU parallel computing allows
 - Drastic reduction in "time to discovery"
 - 1st principle-based simulation at meaningful scale
 - New, 3rd paradigm for research: computational experimentation
- The "democratization" of power to discover
 - \$1000/Teraflops in personal computers today
 - Cost will no longer be the main barrier for big science