GPU Progress and Directions for Earth System Modeling



Stan Posey, sposey@nvidia.com
NVIDIA, Santa Clara, CA, USA



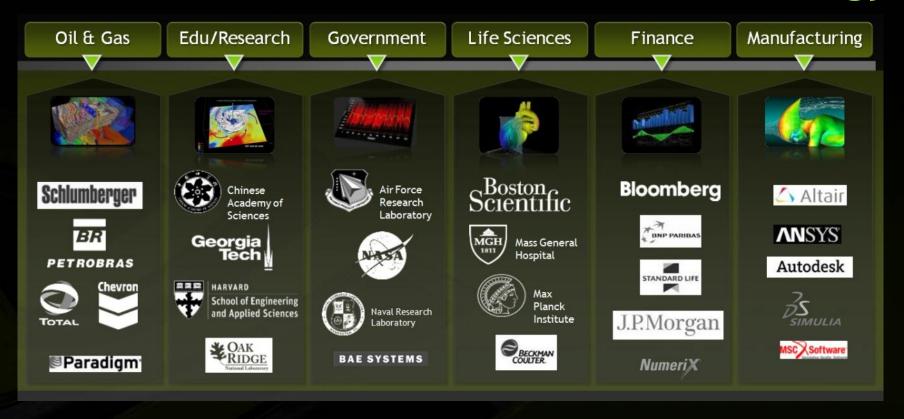


Introduction of GPUs in HPC

- NVIDIA Application Strategy
- GPU Progress in ES Modeling
- NVIDIA Technology Directions

GPU Growth as Mainstream HPC Technology





The buyer plans for including accelerators in their next technical computing server purchase has more than doubled from 29% to over 65% in last 20 months.

IDC Market Research April, 2013

All Major OEM Servers Offer NVIDIA GPUs





Schematic of GPU Accelerated Computing



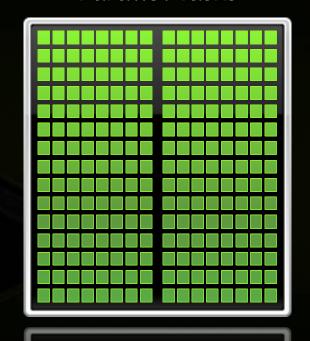


Optimized for Serial Tasks



GPU Accelerator

Optimized for Parallel Tasks

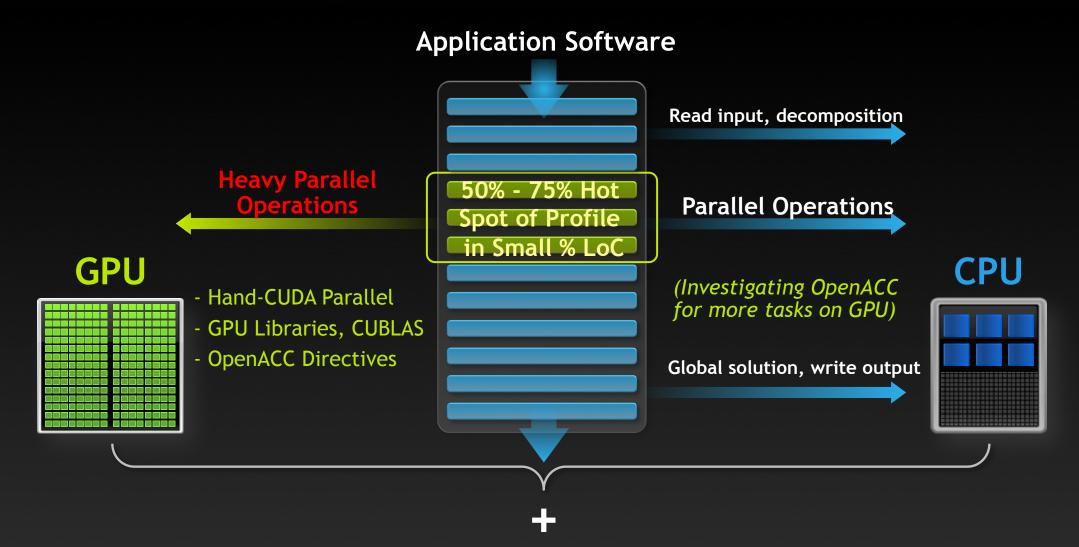


10x PeakPerformance

5x Energy Efficiency

How Applications Are Usually Accelerated



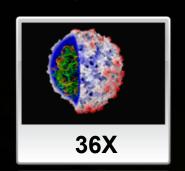


NVIDIA HPC Marketing ~2009 . . .

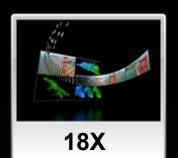




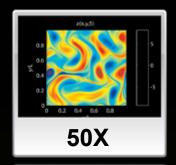
Medical Imaging
U of Utah



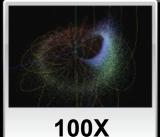
Molecular Dynamics U of Illinois, Urbana



Video Transcoding Elemental Tech

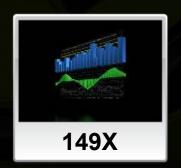


Matlab Computing AccelerEyes



Astrophysics RIKEN

Real Application Speedups



Financial Simulation
Oxford



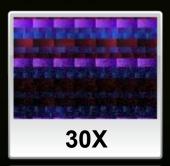
Linear Algebra Universidad Jaime



3D Ultrasound Techniscan



Quantum Chemistry U of Illinois, Urbana



Gene Sequencing
U of Maryland







100X

Astrophysics RIKEN

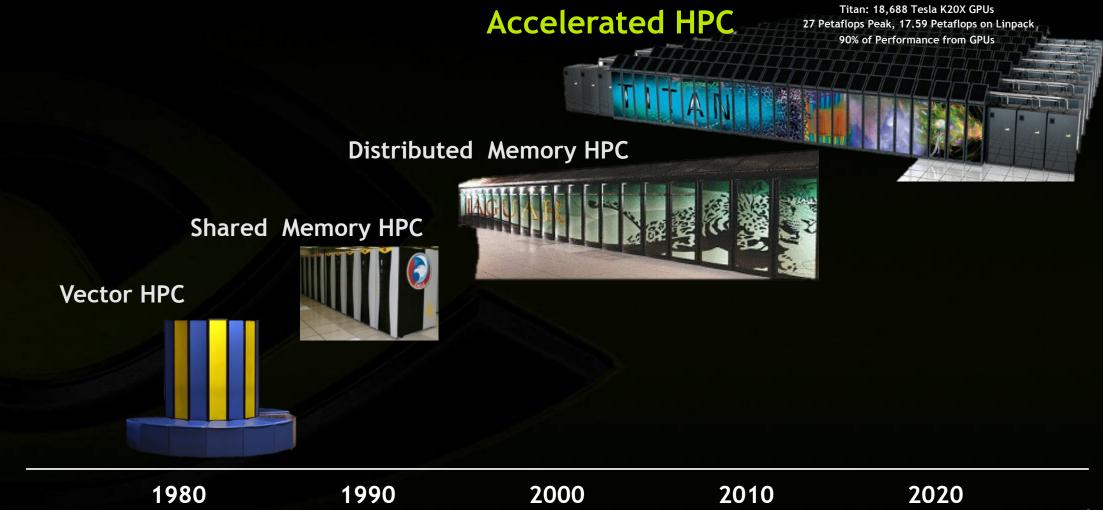
- Full application? Often kernel only without data transfer . . .
- What is the reference CPU? Often old and dusty x86 . . .
- How many CPU cores in the comparison?

149X Often 1 core . . . but who uses only 1 core nowadays?

Financial Simulation Linear Algebra 3D Illtrasound Quantum Chemistry Gene Sequencing NOTE: Missing context often fault of NVIDIA and not the organizations referenced Viand

Next Migration Underway: Accelerated HPC





GPU-Driven Fast and Energy Efficient HPC



TITAN at ORNL

World's Fastest Open Science Supercomputer

18,688 Tesla K20X GPU Accelerators

27 Petaflops Peak

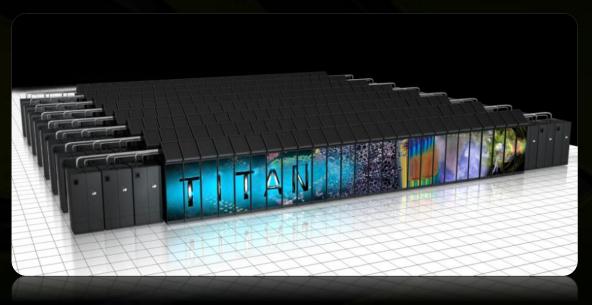
90% of Performance from GPUs

Eurora at CINECA

World's Most Energy Efficient Supercomputer
128 Tesla K20 GPU Accelerators

3150 MFLOPS/Watt

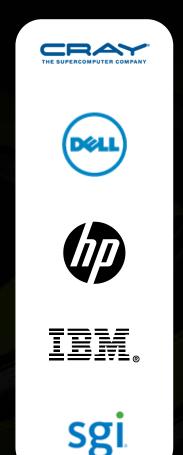
\$100k Energy & 300 Tons of CO₂ Saving Per Year





GPU Acceleration at Leadership HPC Sites





United States

Oak Ridge National Labs
Lawrence Livermore National Labs
Sandia National Labs
NOAA Gaea (ORNL)
NCSA Blue Waters
NCAR Yellowstone (Geyser & Caldera)
NASA Pleadies; Discover

Germany

Juelich HLRS Max Planck TU Dresden

UK

Cambridge EPCC Oxford STFC

Rest of Europe

BSC, Spain CINECA, Italy CEA, France CSCS, Switzerland

Japan

Tokyo Tech RIKEN Tsukuba

China

NSC, Shenzhen NSC, Tianjin CAS IPE

Rest of World

MSU, Russia RAS, Russia IITs, India

Important OEM Collaborations in ES Modeling





Collaboration on large deployments; OpenACC development

■ TITAN —ORNL; Blue Waters —NCSA; Gaea —NOAA/ORNL; Piz Daint —CSCS



Collaboration on strategic deployments; Member Openpower

- Yellowstone NCAR; Discover NASA GSFC
- Openpower Consortium: IBM, NVIDIA, Google, Mellanox, Tyan, others



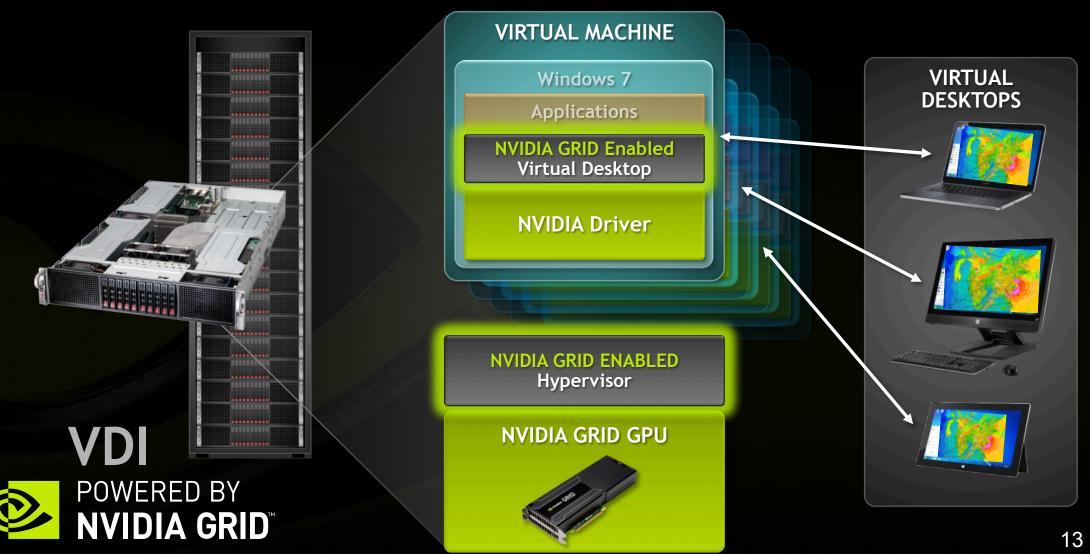
Strategic large deployments including Tsubame - Tokyo Inst of Tech



Strategic deployments including Pleadies – NASA ARC

Remote Visualization With GPU-Driven VDI





GPU Adoption Underway in Data Analytics



Analyzing Twitter



Beyond HPC

GPU-Driven
Big Data

Searching Audio



Visual Shopping



Real-time Video Delivery



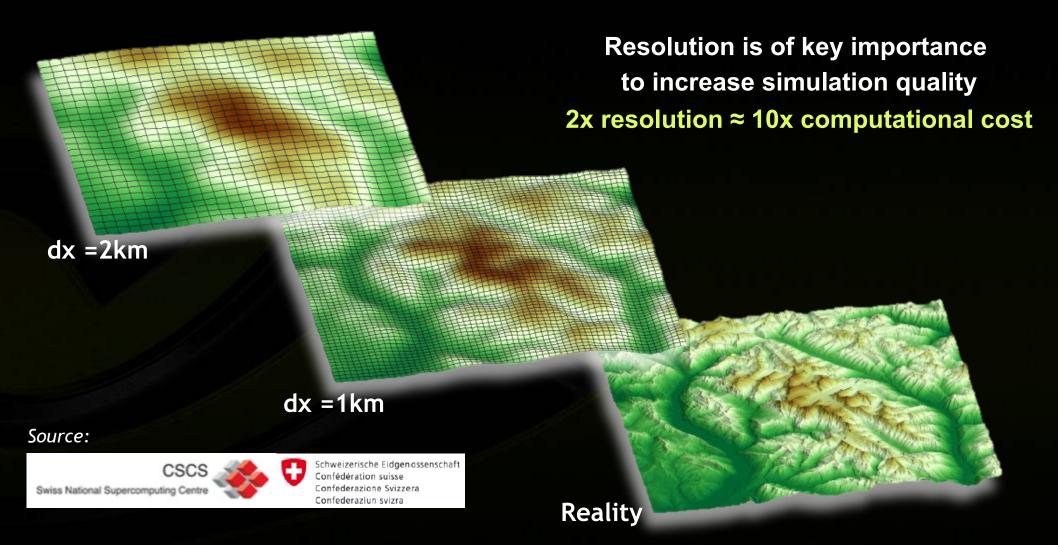




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GPU Motivation: Higher Resolution = High Cost





Example: NASA and Global Cloud Resolving GEOS-6



Programming weather, climate, and earth-system models on heterogeneous multi-core platforms

September 7-8, 2011 at the National Center for Atmospheric Research in Boulder, Colorado



- Dr. William Putman, Global Modeling and Assimilation Office, NASA GSFC



NASA targeting GEOS global model resolution at sub-10-km to 1-km range

Computational requirements for typical 5-day operational forecast:

Grid resolution	Westmere CPU cores	Comments
10 KM	12,000	Possible today
3 KM	300,000	Reasonable but not available
1 KM	10,000,000	Impractical, need acclerators



3.5-km GEOS-5 Simulated Clouds (CPU-Only)

Source: http://data1.gfdl.noaa.gov/multi-core/

NVIDIA Application Strategy Since 2010



- Initial focus on climate and atmospheric research
 - Opportunities to refactor code and use of CUDA
- Later focus on operational models with directives
 - User community imposed Fortran-only requirements
- Direct investments in applications engineering
 - Current collaborations in 6 models and growing
- Continued development in libraries and OpenACC
 - CUBLAS, CUSPARSE, collaborations with PGI, CAPS, Cray
- Collaborations with OEMs (development, benchmarks, etc.)
 - Cray, IBM, HP, SGI, etc.

Programming Strategies for GPU Acceleration



Applications

GPU Libraries

Provides Fast "Drop-In" Acceleration

OpenACC Directives

GPU-acceleration in Standard Language (Fortran, C, C++)

Increasing Development Effort

Programming Languages

Maximum GPU Architecture Flexibility

NVIDIA Application Engineering Investments



	Model	Focus	GPU Approach	Collaboration
WRF	WRF	NWP/Climate	CUDA C, OpenACC	NCAR, Cray, NVIDIA
	COSMO	NWP/Climate	CUDA C, OpenACC	CSCS, SCS, MeteoSwiss, NVIDIA
Stribuid Laboratory	CAM-SE	Climate	CUDA Ftn, OpenACC	ORNL, Cray, NVIDIA
NORA CONTRACTOR OF THE PARTY OF	NIM/FIM	NWP/Climate	F2C-ACC, OpenACC	NOAA, OACC Vendors, NVIDIA
NASA	GEOS-5	Climate	CUDA Ftn, OpenACC	NASA, NVIDIA
NEM@	NEMO	Ocean Model	OpenACC	NVIDIA, STFC (future)

Other Evaluations: GFS, COAMPS, MPAS-A, ROMS; ICON, UKMO GungHo; GRAPES (CN), OLAM (BR)

Other Investments: Government and Research Institutes without direct NVIDIA collaboration

Example: NOPP/ONR Funding in Accelerated HPC





NATIONAL OCEANOGRAPHIC PARTNERSHIP PROGRA



http://www.onr.navy.mil/~/media/Files/Funding-Announcements/BAA/2013/13-011.ashx

ONR BAA13-011:

Advancing Air-Ocean-Land-Ice Global Coupled Prediction on Emerging Computational Architectures

Predictive simulations on heterogeneous architectures Central Processing Unit (CPU), MIC, GPU: identification of representative code patterns that either look particularly amenable or intractable to refactoring; establishment of pathways to maintain single source code compatible with multiple platforms; and determination of mechanisms to achieve optimal performance and portability.

- Total of \$3.75M funding distributed among 4 8 awards (closed Apr 2013)
- Models: GFS, HIRAM, NIM, MOM, CESM, HYCOM, CICE, Wavewatch3, NUMA

Rapid OpenACC Growth Since 2011 Founding



26+ Community Applications

Cloverleaf MiniMD COSMO (Physics) NICAM DNS NIM

> **EMGS ELAN NEMO GYRE**

GAMESS PALM-GPU

Quantum Espresso **GENE**

GEOS RAMSES

GTC ROMS

Harmonie S₃D

> **HBM** Seismic CPML

ICON SPECFEM-3D

LULESH **UPACS**

MiniGhost WRF

S₃D **WRF**

Cloverleaf

COSMO (Physics)

HBM

NIM

2012 2013

HPC Industry Support Grows 2x



CRAY

INVIDIA.

2012



INVIDIA.

2013

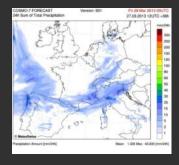


OpenACC in Practice for NWP and Climate



Examples: Use of directives with less effort; ease in maintenance and flexibility



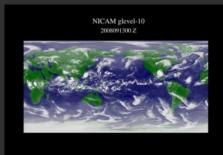


COSMO (Physics)

NWP

- Goal: preserve physics code (22% of runtime), augmenting refactored dynamics in CUDA
- Physics scheme speedup 4.2X vs. multi-core Xeon





NICAM

Climate

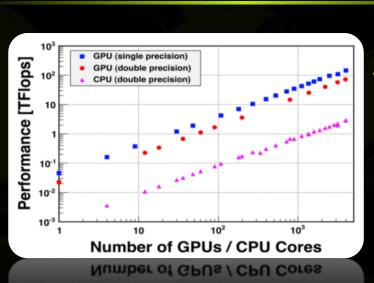
- Hotspots using CUDA, then OpenACC
- CUDA: 3.1x faster on GPU vs. CPU node
- OpenACC: (preliminary)= 69-77% of CUDA
 - More portable, more maintainable
 - Full OpenACC port in progress

TiTech NWP 2010 Achievement: ASUCA 145 TF

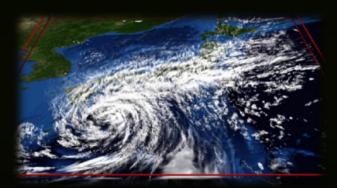


Tsubame 2.0 東京工業大学
Tokyo Institute of Technology
Tokyo Institute of Technology

- 1.19 Petaflops
- 4,224 Tesla M2050 GPUs



3990 Tesla M2050s 145.0 Tflops SP 76.1 Tflops DP

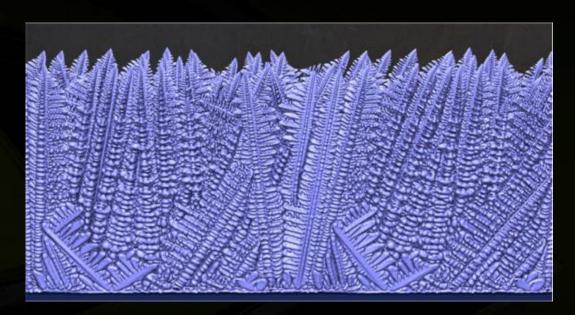


ASUCA and NWP Simulation on Tsubame 2.0, TiTech Supercomputer: Dr. Takayuki Aoki, GSIC, Tokyo Institute of Technology, Tokyo Japan

TiTech Winner of 2011 Gordon Bell Prize



Special Achievement in Scalability and Time-to Solution



"Peta-scale Phase-Field Simulation for Dendritic Solidification on the TSUBAME 2.0 Supercomputer" -- T. Shimokawabe, T. Aoki, et. al.

Tsubame 2.0 Tokyo Institute of Technology



2,816 x86 CPUs





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WRF

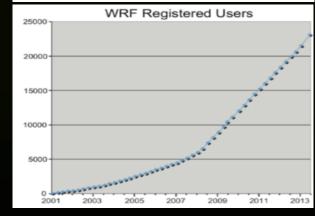
- http://irina.eas.gatech.edu/EAS8802_Spring2011/Lecture7.pdf
- http://www.mmm.ucar.edu/wrf/users/workshops/WS2010/presentations/Lectures/Microphysics10.pdf
- http://www.mmm.ucar.edu/wrf/users/docs/user_guide_V3.1/users_guide_chap5.htm#_Installing_WRF
- http://www.mmm.ucar.edu/wrf/WG2/GPU/WSM5.htm
- Jarno Mielikainen, Bormin Huang, Hung-Lung Allen Huang, and Mitchell D, Goldberg, "Improved GPU/CUDA Based Parallel Weather and Research Forecast(WRF) Single Moment 5-Class (WSM5) Cloud Microphysics", IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing, Vol 5, No.4, August 2012

WRF: Operational in 21 Countries; 153 Total





Registered Users	5
U.S. Universities	3,600
U. S. Gov't labs, Private sector	3,591
Foreign users	15,916
	23,107
Countries represente	ed: 153



Source: Welcome Remarks, 14th Annual WRF Users' Workshop, 24-28 Jun 2013, Boulder, CO

GPU Status of WRF Developments



- Several non-trunk efforts at various stages:
 - 2009: Physics schemes by John Michalakes: www.mmm.ucar.edu/wrf/WG2/GPU/
 - 2010: Dynamics and some physics by Thomas Nipen at UBC source at NVIDIA
 - 2011: Shortwave radiation model by NVIDIA (G. Ruetsch) and PGI (available)
 - 2012: C-DAC and HPC-FTE group working with NVIDIA India Developers
 - **2012:** NOAA announced NIM dycore with WRF physics, but now GFS and YSU
 - 2012: Cray and OpenACC (Pete Johnsen) results at NCAR multi-core workshop
 - Ongoing: KernelGen project: www.kernelgen.org update at NVIDIA GTC 2013
 - Ongoing: 50% of physics schemes by Space Science Engineering Center, UW-M
- Trunk efforts at various stages:
 - WSM5 physics model (15% 25%) in release 3.2 from 2009 (now dormant)
 - WRF 3.5 with OpenACC –NVIDIA and NCAR (MMM Dave Gill) collaboration

OpenACC Developments for WRF 3.4/3.5



Programming weather, climate, and earth-system models on heterogeneous multi-core platforms

September 12-13, 2012 at the National Center for Atmospheric Research in Boulder, Colorado

WRF Experiments on GPU
Accelerators using OpenACC

- Pete Johnsen, Cray, Inc.

WRF routine advance w

- Dynamics routine to advance vertical velocity
- Standard Fortran use with OpenACC directives
- 2.1x speedup for 16 cores

advance w Results WRF advance w Kernel Performance 2.1x speedup over 16 Interlagos cores. 35 11.6x speedup over single Data transfer not included. 15 8 AMD cores 4 AMD cores 12 AMD cores

Source: http://data1.gfdl.noaa.gov/multi-core/

Published WRF Speedups from SSEC

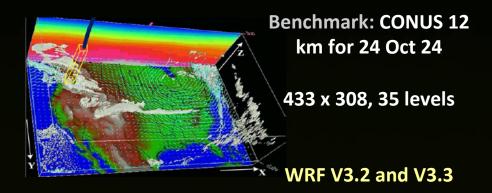




WRF Module name	Speedup
Single moment 6-class microphysics	500x
Eta microphysics	272x
Purdue Lin microphysics	692x
Stony-Brook University 5-class microphysics	896x
Betts-Miller-Janjic convection	105x
Kessler microphysics	816x
New Goddard shortwave radiance	134x
Single moment 3-class microphysics	331x
New Thompson microphysics	153x
Double moment 6-class microphysics	206x
Dudhia shortwave radiance	409x
Goddard microphysics	1311x
Double moment 5-class microphysics	206x
Total Energy Mass Flux surface layer	214x
Mellor-Yamada Nakanishi Niino surface layer	113x
Single moment 5-class microphysics	350x
Yonsei University planetary boundary layer scheme	108x
5-Layer Thermal diffusion land surface layer	211x
Pleim-Xiu surface layer	665x
•	

Hardware: Core-i7 3930K, 1 core use; GTX 590 GeForce





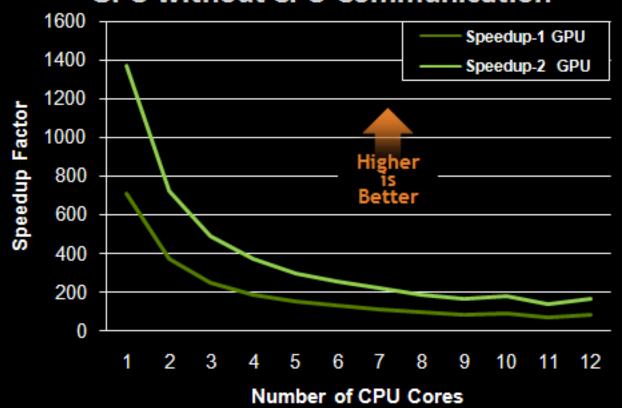
Verification: WSM5 by NREL (J. Michalakes) and NVIDIA Applications Engr [Next 2 slides]

NOTE: All times without CPU data transfer

NVIDIA Verification of WSM5 from SSEC



WRF WSM5 for CONUS 12KM; GPU without CPU Communication





2 x Core-i7 3930K, Total of 12 Cores; GPUs: 2 x Tesla K20X



Benchmark: CONUS 12 km resolution for October 24, 2001;

433 x 308 grid points,
35 vertical levels

NOTE: Times with no CPU data transfer

NREL Verification of WSM5 from SSEC



High performance computing enhancements to WRFV3.5

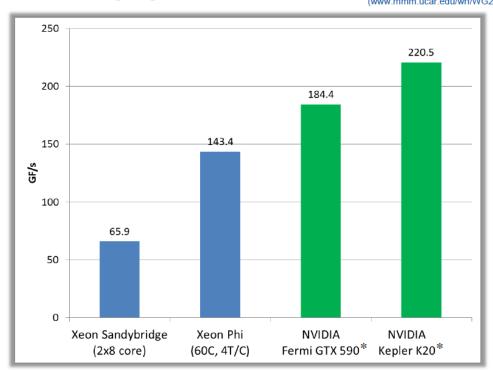
- John Michalakes, National Renewable Energy Laboratory, USA www.mmm.ucar.edu/wrf/users/workshops/WS2013/WorkshopPapers.php



WSM5 Microphysics

WSM5 CONUS 12KM Workload, 6.53 GF/call (Intel SDE) (www.mmm.ucar.edu/wrf/WG2/bench)





^{*} Improved GPU/CUDA Based Parallel Weather and Research Forecast (WRF) Single Moment 5-Class (WSM5) Cloud Microphysics.

J. Mielikainen, B. Huang, H-L. A. Huang, and M.D. Goldberg. IEEE JSTARS, Vol. 5, No. 4, Aug. 2012 and personal communication

14th Annual WRF Users' Workshop, 24 – 26 Jun 2013, Boulder, CO, USA

- GigaFlop ratings of WSM5
 Thompson microphysics
 scheme (not a full model run)
- Data transfer times with CPU excluded in all results

Performance Results

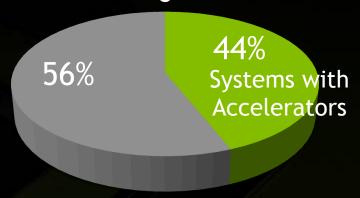
K20X GPU vs. CPU = 3.34x

K20X GPU vs. Phi = 1.54x

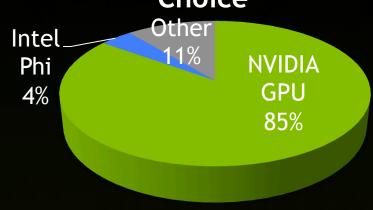
GPU Accelerated Computing Growing Fast



44% Systems Now Have Accelerators











"Intel is not taking share away from NVIDIA but rather both are expanding the use of accelerators."

Intersect360 Research

HPC User Site Census July, 2013

Accelerator Progress Reports at NCAR Workshop



Programming weather, climate, and earth-system models on heterogeneous multi-core platforms

September 19-20, 2013 at the National Center for Atmospheric Research in Boulder, Colorado

Session: Focus:

Session 1 - Common Features and Challenges of Using Multi-core Systems	CPU
Session 2 - Optimization for Hybrid GPU systems	GPU
Session 3a - Porting and Optimizing for Intel Xeon and Xeon Phi	Phi
Session 3b - Porting and Optimizing for Intel Xeon and Xeon Phi	Phi
Session 4 - Common Features and Challenges of Using Multi-core Systems	CPU
Session 5 - Porting and Optimizing for Intel Xeon and Xeon Phi	Phi
Session 6a - Optimizing for GPUs using CUDA and OpenACC	GPU
Session 6b - Optimizing for GPUs using CUDA and OpenACC	GPU

Organizers

Ilene Carpenter (NREL), Mark Govett (ESRL), Chris Kerr (GFDL), Rich Loft (NCAR), Bill Putman (GSFC), William Sawyer (CSCS)





Running the FIM and NIM Weather Models on GPUs

- Mark Govett (NOAA Earth System Research Laboratory)

Source: http://on-demand.gputechconf.com/gtc/2013/presentations/S3429-FIM-NIM-Weather-Models-on-GPUs.pdf



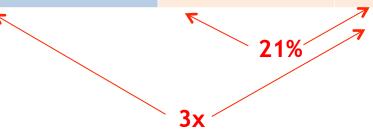
NIM Serial Performance (2013)



- No changes to the source code
- Single Socket Performance
 - 10K horizontal points, 96 vertical levels
- Very efficient CPU performance
 - Measured 29% of peak performance (Intel Westmere)

NIM	Opteron	Westmere	SandyBridge	Fermi	K20x
runtime	143.0	86.8	60.0	25.0	20.7

- Parallel performance
 - Being run on up to 160 GPUs
 - Working on optimizing inter-GPU communications





NIM Parallel Performance



- Weak Scaling with Communications Optimization
 - Moved collective operation to the CPU instead of doing it on the GPU using GPU MappedMemory
 - Too many small writes across the PCle bus
 - Resulted in a 5-17x speedup for the Pack Operation

GPUs	GPU to GPU Comm Time	Total Time Time (sec)	
10	232 (22%)	1034	
40	247 (23%)	1054	
160	266 (24%)	1076	

Operation	Time		
Iniitilalization	3	(1%)	
Pack Data on GPU	45	(17%)	
CPU – GPU Copy	59	(22%)	
MPI Comms	82	(31%)	
UnPack on GPU	77	(29%)	
Total	266		



3.5KM NIM on Titan in 2013



Dynamics on GPU, Physics on CPU + OMP for now



10 day forecast, 10,262 horizontal points / GPU

Resolution KM	Vertical Levels	GPUs	Dynamics Time	CPU-GPU Transfer	Physics Time	Total Time In Hours
30	96	80	1700	400	1900	1.1
15	96	320	1700	400	1900	2.2
7.5	96	1280	1700	400	1900	4.4 (1.8%)
3.75	96	5120	1700	400	1900	8.8 (3.6%)



NEMO

Accelerating NEMO with OpenACC

- Maxim Milakov (NVIDIA)

Source: http://on-demand.gputechconf.com/gtc/2013/presentations/S3209-Accelerating-NEMO-with-OpenACC.pdf

NEMO Acceleration Using OpenACC





Background

- NEMO ocean modeling framework: http://www.nemo-ocean.eu/
- Used by 240 projects in 27 countries (14 in Europe, 13 elsewhere)

Approach

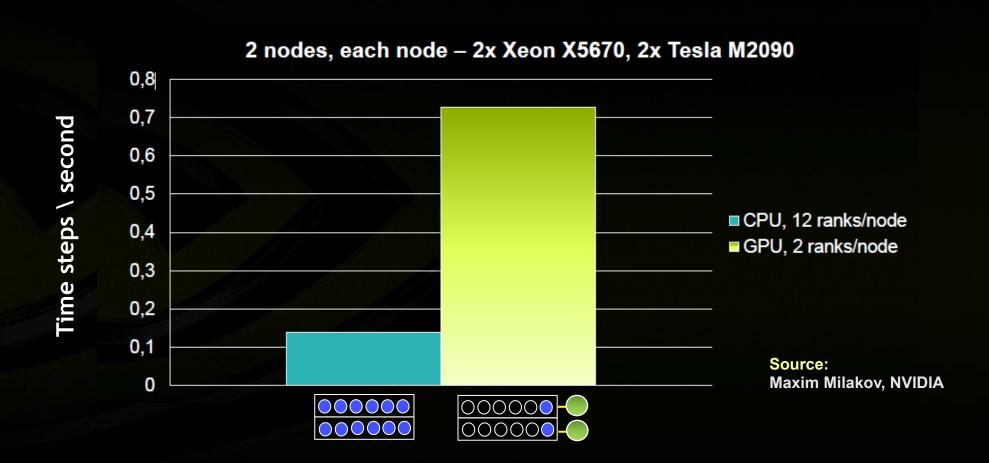
- Project based on NEMO 3.4, use of PGI Fortran compiler 12.9 preview
- Flat profile, 1st routine is 6%, many routines to accelerate for overall benefit
- OpenACC "present" clause keeps data on the device between subroutine calls
- Directives for 41 routines: rearranged loops in 12, temporary arrays in 13
- Other changes for improved MPI communication, other miscellaneous

NEMO Acceleration Using OpenACC





GYRE_50 Configuration, I/O disabled, OpenACC 1.0: Speedup ~5x

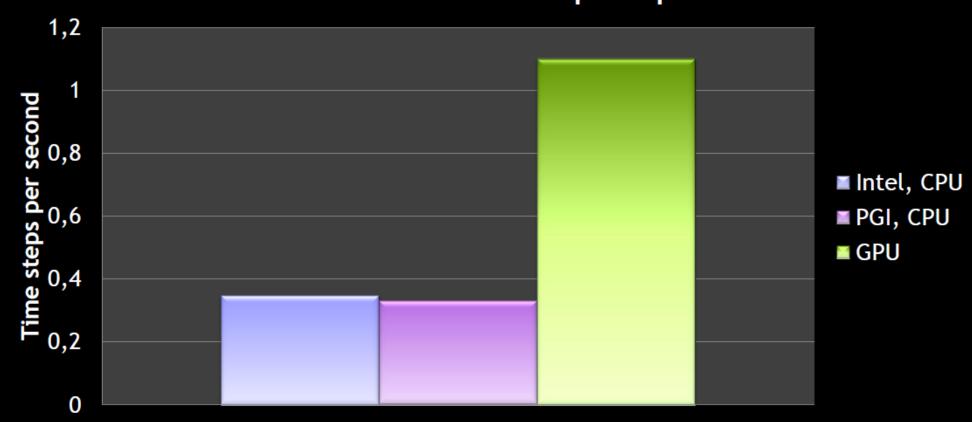


Benchmarking - hardware

- "Sandy Bridge + Kepler" nodes, each having:
 - CPU: 2 sockets * Xeon E5-2670 (Sandybridge), 2.6GHz (3.3GHz Turbo Boost), 8 cores, 64 GB RAM
 - GPU: 2x Tesla K20X, ECC off, 6GB RAM each
 - 4x FDR Infiniband (56 Gb/s)
- Running configuration is GYRE_50 (1/4 degree), requires about 23GB of total RAM, fits 4 K20X
- The code is running on 2 nodes
- The performance is measured by running 1000 time steps,
 startup and shutdown overheads are not included in figures

Benchmarking - results

GPU vs. CPU - 3.1x speedup



. .





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Tesla Kepler Family



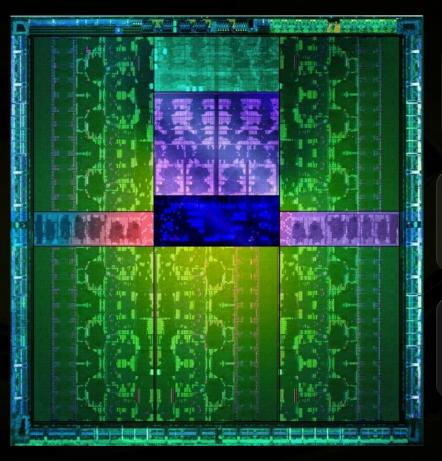
World's Fastest and Most Efficient HPC Accelerators

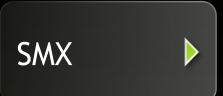
● INVIDIA TESLA	GPUs	Single Precision Peak (SGEMM)	Double Precision Peak (DGEMM)	Memory Size	Memory Bandwidth (ECC off)	System Solution
Weather & Climate,	K20X	3.95 TF (2.90 TF)	1.32 TF (1.22 TF)	6 GB	250 GB/s	Server only
Physics, BioChemistry, CAE, Material Science	K20	3.52 TF (2.61 TF)	1.17 TF (1.10 TF)	5 GB	208 GB/s	Server + Workstation
Image, Signal, Video, Seismic	K10	4.58 TF	0.19 TF	8 GB (4 GB ea.)	320 GB/s	Server only

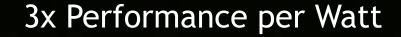


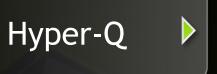


Fastest, Most Efficient HPC Architecture Ever









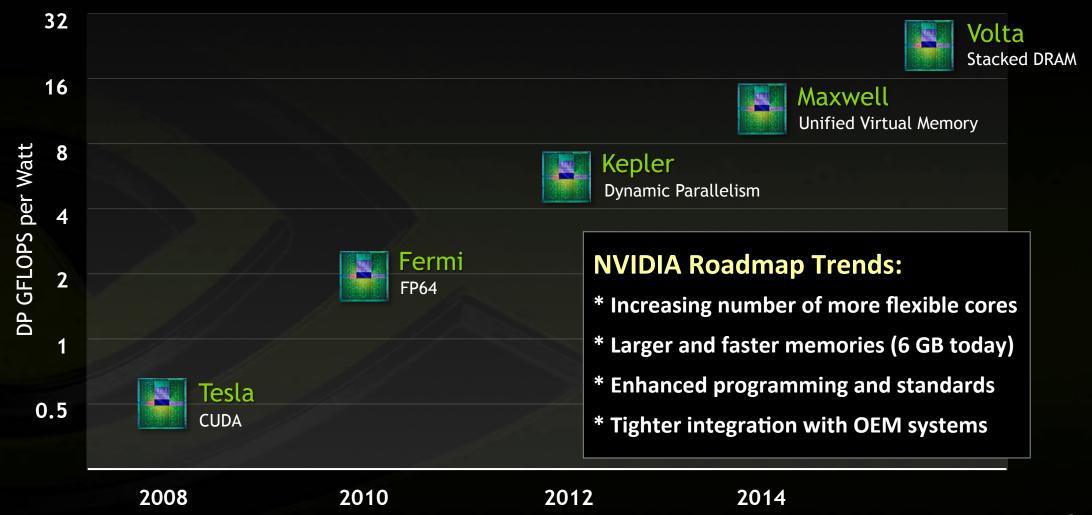
Easy Speed-up for Legacy MPI Apps



Parallel Programming Made Easier than Ever

NVIDIA GPU Roadmap (Details Require NDA)





ARM Support Now Available Since CUDA 5.5



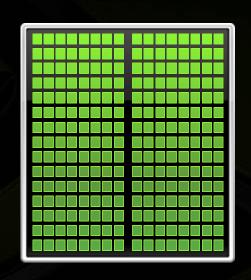
ARM or x86 CPU

Optimized for Few Serial Tasks



Optimized for Many Parallel Tasks





CUDA 5.5 Highlights

Full Support for ARM Platforms

Native compilation on ARM

Optimized for MPI

- Faster Hyper-Q for all Linux distros
- MPI workload prioritization

Guided Performance Analysis

Step-by-step optimization

Available Now

http://developer.nvidia.com/cuda-toolkit

NVIDIA Quadro K6000: Kepler-Based 12GB GPU





Announced July 2013

Available Q3 2013

http://www.nvidia.com/object/quadro-desktop-gpus.html

QUADRO K6000 QUICK SPECS				
CUDA Parallel-Processing Cores	2880			
Frame Buffer Memory	12 GB GDDR5			
Max Power Consumption	225 W			
Graphics Bus	PCI Express 3.0 x16			
Display Connectors	DVI-I (1), DVI-D (1) DP 1.2 (2), Optional Stereo (1)			
Form Factor	4.376" H x 10.5" L Dual Slot			

Summary For GPUs and ES Modeling



- Opportunities exist for GPUs to provide significant performance acceleration for ES Models
 - Improved simulation quality from higher resolutions
 - Faster time to predictions for operational forecasting
 - Cut down energy consumption in IT procedures
- Simulations recently considered intractable are now possible
 - Global models are cloud resolving scale
 - Parameter physics at higher resolutions and more frequent time steps
 - Expanded and more common use of ensembles

Thank you & Questions



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