GPU Considerations of ESMs for the Pre-Exascale HPC Phase

Stan Posey; <u>sposey@nvidia.com</u>; NVIDIA, Santa Clara, CA, USA HPC Program Manager, ESM and CFD Solutions Agenda: Application Readiness for the Pre-Exascale Phase



NVIDIA Update and HPC Trends

Developments in Pre-Exascale HPC

ESM Requirements and GPU Progress

NVIDIA Core Technologies and Markets



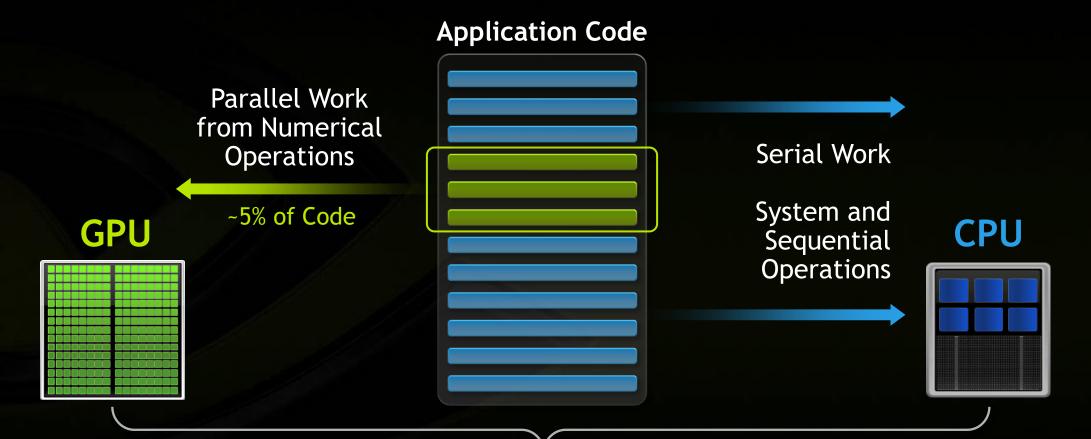
Company Revenue of ~\$5B USD; ~9,000 Employees; HPC Growing > 30% CAGR







Optimization of Serial + Parallel Execution

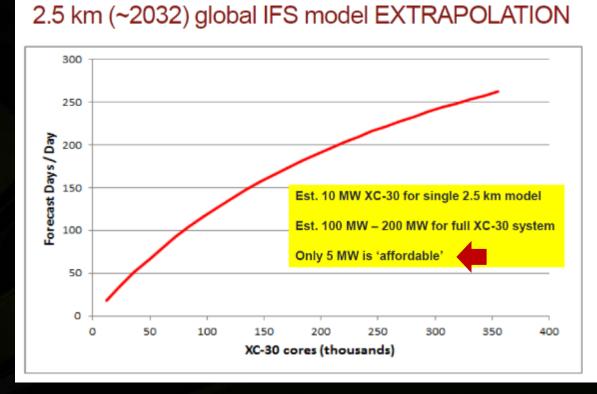


GPU Motivation (II): Power Limiting Trends



Challenges of Getting ECMWF's Weather Forecast Model (IFS) to the Exascale

– G. Mozdzynski, ECMWF 16th HPC Workshop



"Conclusion: Current mathematics, algorithms and hardware will not be sufficient (by far)"

GPU Motivation (III): ES Model Trends



- Higher grid resolution with manageable compute and energy costs
 - Global atmosphere models from 10 km today to cloud-resolving scales of 1-3 km



Increase in ensemble use and ensemble members to manage uncertainty



Fewer model approximations (NH), more features (physics, chemistry, etc.)

Accelerator technology identified as a cost-effective and practical approach to future NWP requirements

Tesla GPU Progression During Recent Years

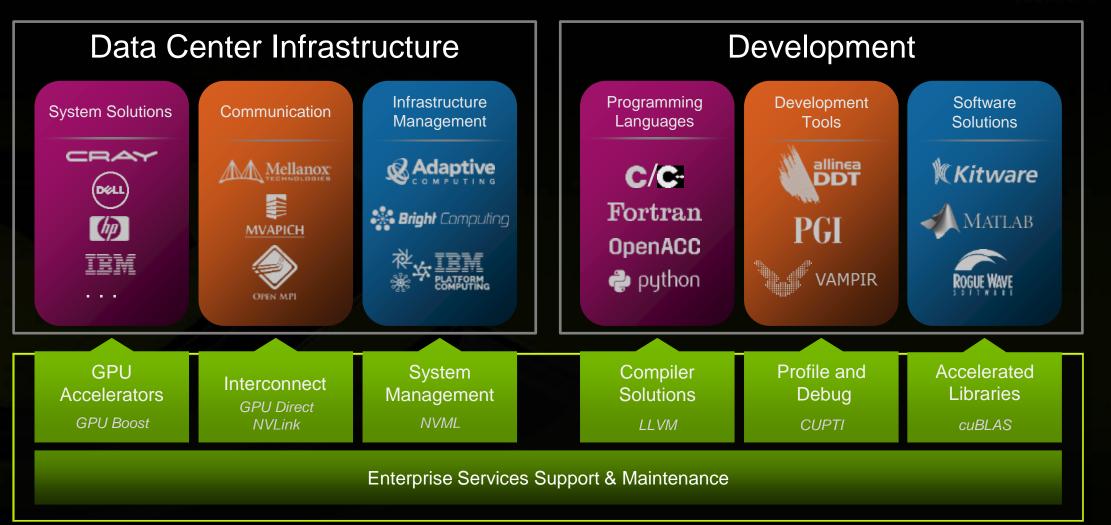


and the second	2012 (Fermi) M2075	2014 (Kepler) K20X	2014 (Kepler) K40	2014 (Kepler) K80	Kepler / Fermi
Peak SP Peak SGEMM	1.03 TF	3.93 TF 2.95 TF	4.29 TF 3.22 TF	8.74 TF	4x
Peak DP Peak DGEMM	.515 TF	1.31 TF 1.22 TF	1.43 TF 1.33 TF	2.90 TF	3х
Memory size	6 GB	6 GB	12 GB	24 GB (12 each)	2x
Mem BW (ECC off)	150 GB/s	250 GB/s	288 GB/s	480 GB/s (240 each)	2x
Memory Clock		2.6 GHz	3.0 GHz	3.0 GHz	
PCIe Gen	Gen 2	Gen 2	Gen 3	Gen 3	2x
# of Cores	448	2688	2880	4992 (2496 each)	5x
Board Power	235W	235W	235W	300W	0% – 28%

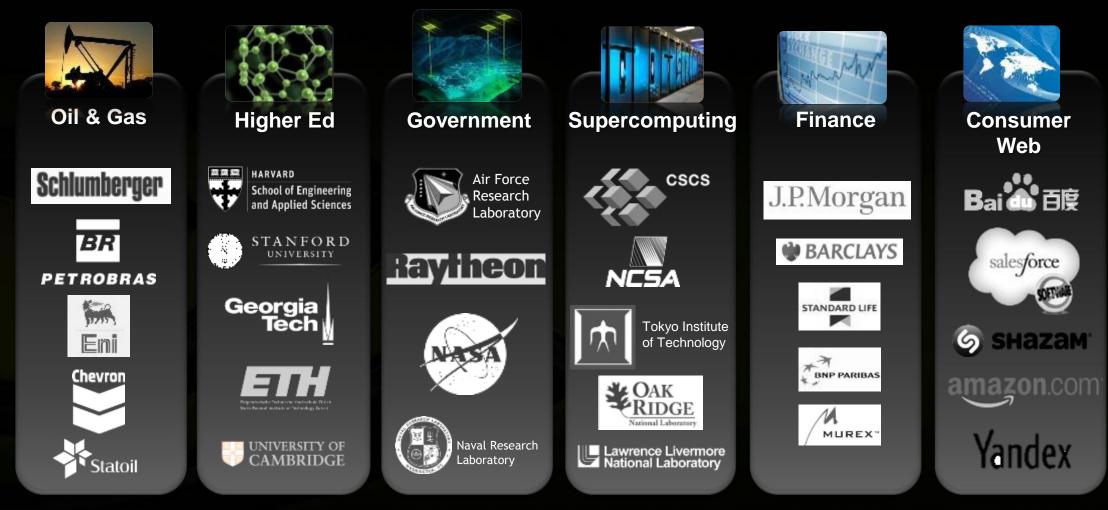
Note: Tesla K80 specifications are shown as aggregate of two GPUs on a single board

GPU Technology a Mainstream HPC Platform





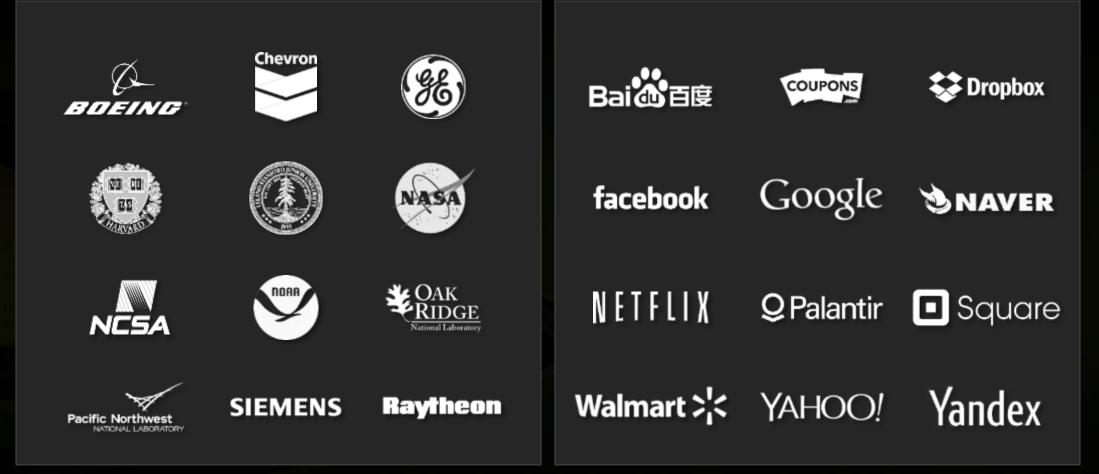
GPUs Applied Across Mainstream HPC Domains

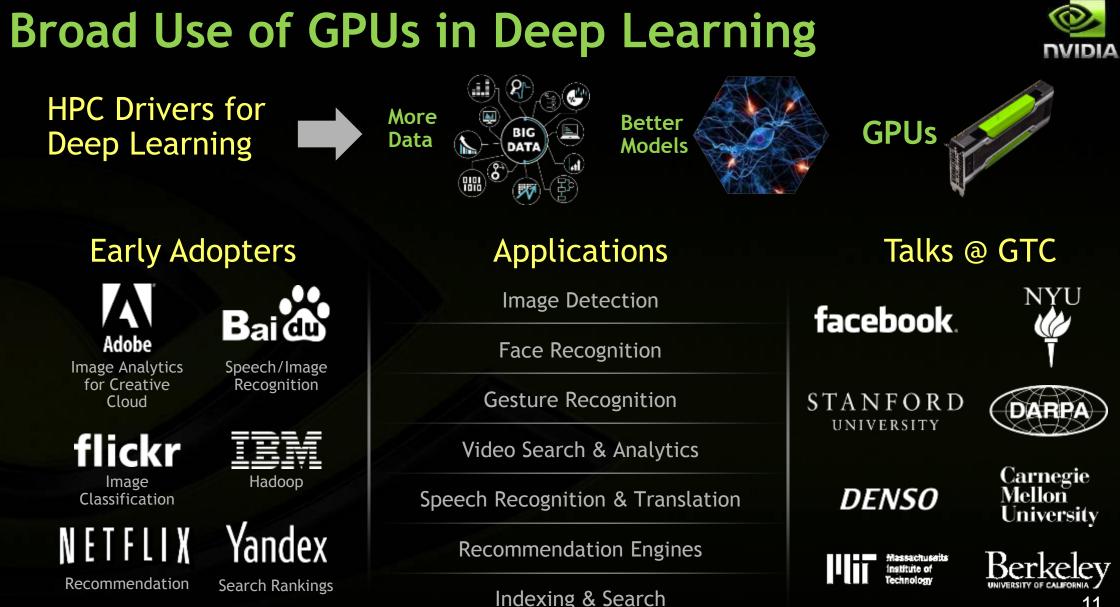


GPUs Expanding from HPC to Data Analytics



Attendees at NVIDIA GPU Technology Conference (GTC) 2014





NVIDIA Invited to Participate in CI2015



Software * Data Portals * User Support * Resources *

About Us



NCAR

UCAR

5th International Workshop on Climate Informatics September 24-25, 2015

Hosted by the National Center for Atmospheric Research in Boulder, CO

CI2015 - Agenda

September 25, 2015, NCAR, MSR

Computational & Information Systems Lab

- 8:30 9:30 Invited Talk Rich Caruana: Do Deep Nets Really Need To Be Deep?
- 9:30 10:15 Panel Discussion: Deep Learning for Climate Science
- 10:45 11:45 **Invited Talk Imme Ebert-Uphoff:** Knowledge discovery in climate science
- 1:00 2:00 Invited Talk Yolanda Gil: Intelligent Systems for Climate Research: When Will Deep Learners Meet Deep Knowledge?

5th Intl Workshop on Climate Informatics, 24 – 25 Sep, 2015 NCAR, Boulder, USA

Growing Agenda

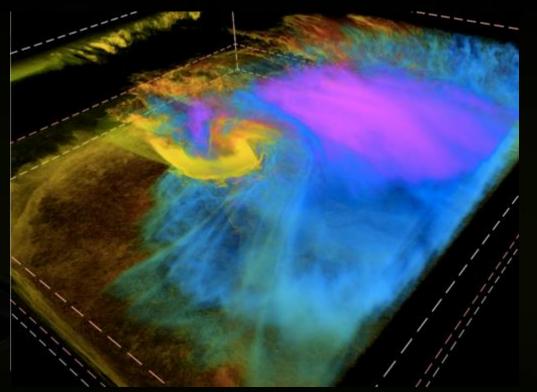
on Deep Learning

Index: Scalable Rendering for Volume Visualization

- Leverages GPU-clusters for largescale (volume) data visualization and interactive visual computing
 - Commercial software solution available and deployed for in-situ visualization of large-scale data
 - Plugin for ParaView under development and available soon

http://www.nvidia-arc.com/products/nvidia-index.html

1.8 billion cells + 500 time steps



Dataset courtesy of Prof. Leigh Orf, UW-Madison and Rob Sisneros, NCSA

Agenda: Application Readiness for the Pre-Exascale Phase



NVIDIA Update and HPC Trends

Developments in Pre-Exascale HPC

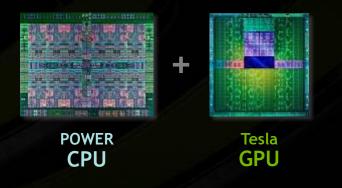
ESM Requirements and GPU Progress

IBM Power + NVIDIA GPU Accelerated HPC



Next-Gen IBM Supercomputers and Enterprise Servers

Long term roadmap integration



OpenPOWER Foundation

Open ecosystem built on Power Architecture

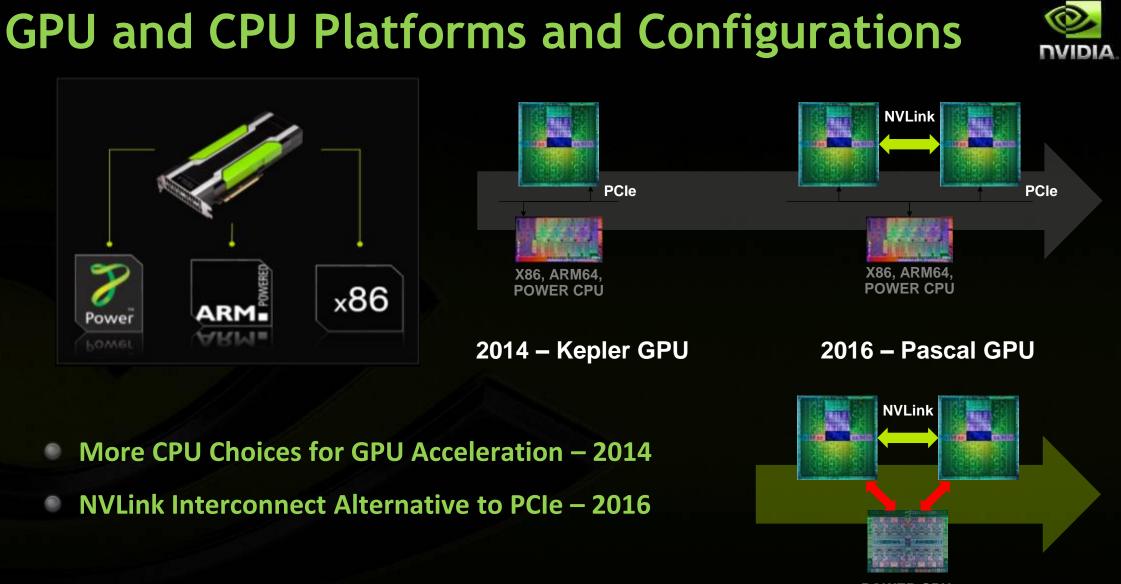








First GPU-Accelerated POWER-Based Systems Available Since 2015



Features of Pascal GPU Architecture – 2016

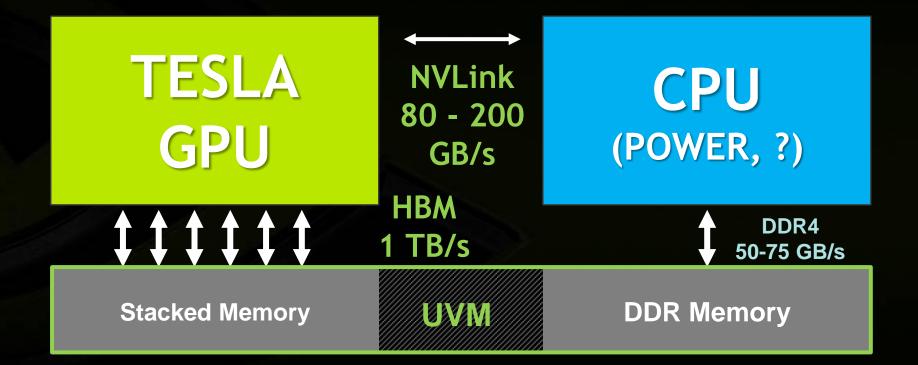
NVLink Interconnect at 80 GB/s (Speed of CPU Memory)

Stacked Memory

4x Higher Bandwidth ~1 TB/s 3x Capacity, 4x More Efficient

Unified Memory

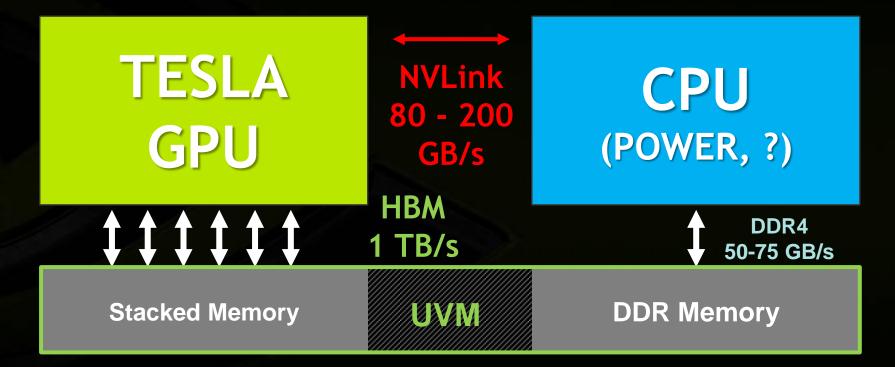
Lower Development Effort (Available Today in CUDA6)



NVLink Interconnect Alternative to PCIe



- High speed interconnect for CPU-to-GPU and GPU-to-GPU
- Performance advantage over PCIe Gen-3 (5x to 12x faster)
- GPUs and CPUs share data structures at CPU memory speeds



NVLink Interconnect Alternative to PCIe



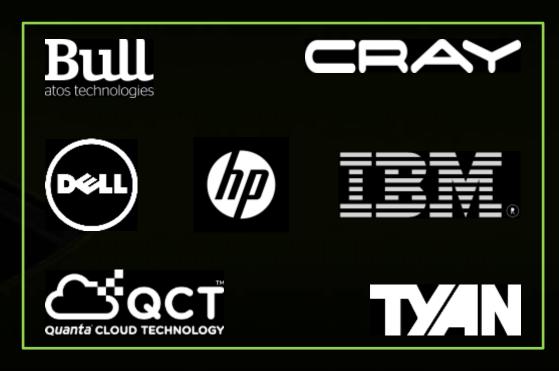




HP SL270: 8 x K80

HPC Vendors & NVLink-2016

- All will support GPU-to-GPU
- Several to support CPU-to-GPU





US DOE Pre-Exascale Phase Deployment in 2017

US DOE CORAL Systems

- Summit (ORNL) and Sierra (LLNL)
- Installation 2017 at ~150 PF each
- Nodes of POWER 9 + Tesla Volta GPUs
- NVLink Interconnect for CPUs + GPUs

ORNL Summit System

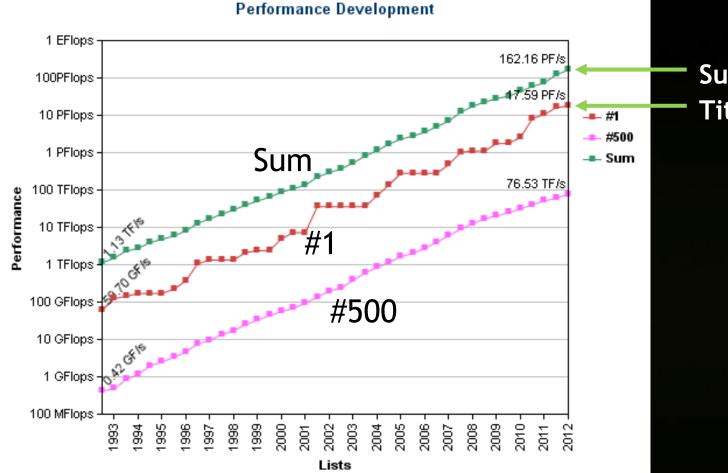
- Approximately 3,400 total nodes
- Each node 40+ TF peak performance
- About 1/5 of total #2 Titan nodes (18K+)
- Same energy used as #2 Titan (27 PF)



1/5th the Nodes, Same Energy Use as Titan

Summit System Relative to HPC Top 500





Summit System Titan System

> Summit will have same capacity as <u>all Top500 systems</u> on the list in 2012 combined — same year Titan was #1

Feature Comparison of Summit vs. Titan



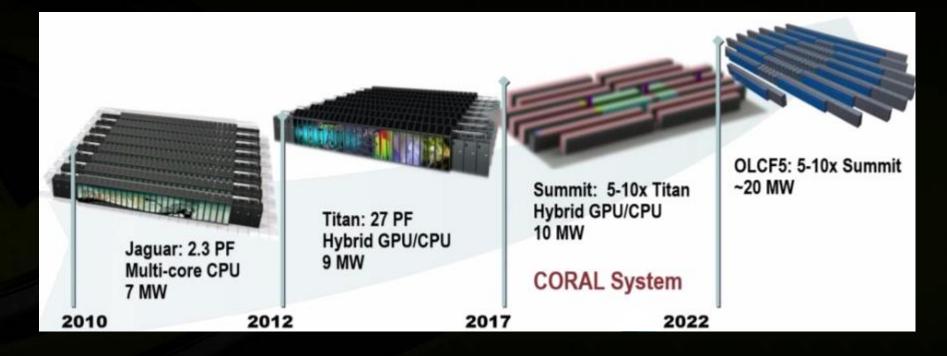
Feature	2017 Summit	2012 Titan	
Application Performance	5-10x Titan	Baseline	~5 - 1
Number of Nodes	~3,400	18,688	~1/!
Node performance	> 40 TF	1.4 TF	~30
Memory per Node	>512 GB (HBM + DDR4)	38GB (GDDR5+DDR3)	~15
NVRAM per Node	800 GB	0	
Node Interconnect	NVLink (5-12x PCle 3)	PCIe 2	~10 -
System Interconnect (node injection bandwidth)	Dual Rail EDR-IB (23 GB/s)	Gemini (6.4 GB/s)	
Interconnect Topology	Non-blocking Fat Tree	3D Torus	
Processors	IBM POWER9 NVIDIA Volta™	AMD Opteron™ NVIDIA Kepler™	
File System	120 PB, 1 TB/s, GPFS™	32 PB, 1 TB/s, Lustre®	
Peak power consumption	10 MW	9 MW	~0>

x

US DOE Projections of Exascale by 2022



Present and Future Leadership Computers at OCLF – J. Wells, GTC 2015



Agenda: Application Readiness for the Pre-Exascale Phase



NVIDIA Update and HPC Trends

Developments in Pre-Exascale HPC

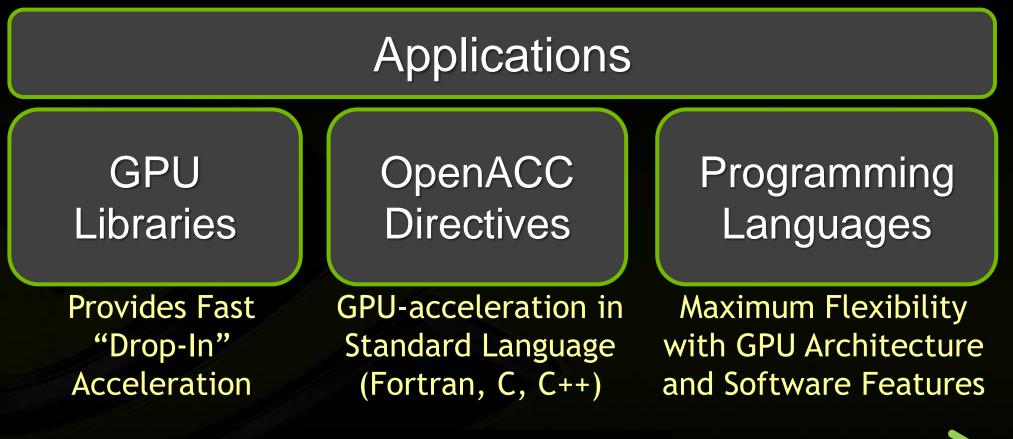
ESM Requirements and GPU Progress

ESM Characteristics and GPU Considerations



- Flat execution profiles no real 'hot spots'
 - Programming models must enable optimization-everywhere for GPUs
- Large Fortran code base with a 'community' of developers
 Usually restricts some portion of the code/model to directives approach
- Dynamical cores distributed parallel with frequent communication
 Fast interconnects, GPU-aware MPI with direct GPU-to-GPU communication
- Development environment for multi-level parallelism
 Libraries, tools, debuggers, compilers for OpenMP and OpenACC
- Data center infrastructure and system mgmt (vs. card 'plug-in')
 - Vendor collaboration/integration (Cray, IBM, SGI, Bull, HP, Lenovo, etc.)





Increasing Development Effort

NOTE: Many application developments include a combination of these strategies

NVIDIA GPU Focus for Atmosphere Models



Global

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Organization	Location	Model	GPU Approach
ORNL, SNL	US	CAM-SE	OpenACC (migration from CUDA-F)
NOAA ESRL	US	FIM/NIM	OpenACC, F2C-ACC
NASA GSFC	US	GEOS-5	OpenACC (migration from CUDA-F)
NCAR MMM	US	MPAS-A	OpenACC
NOAA GFDL	US	FV3	OpenACC
ECMWF	UK	IFS (Arpege)	Libs + OpenACC
STFC, MetOffice	UK	UM/GungHo	OpenACC
CSCS, MPI-M	CH, DE	ICON	DSL – dycore, OpenACC – physics
JAMSTEC, UT, RIKE	I JP	NICAM	OpenACC
(i) NCAR; (ii) SSEC	US	WRF-ARW	(i) OpenACC, (ii) CUDA
MCH, CSCS	СН	COSMO	DSL – dycore, OpenACC – physics
Bull	FR	HARMONIE	OpenACC
TiTech	JP	ASUCA	Hybrid-Fortran, OpenACC

NVIDIA GPU Focus for Atmosphere Models

JP

TiTech



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Organization	Location	Model	GPU Approach
ORNL, SNL	US	CAM-SE	OpenACC (migration from CUDA-F)
NOAA ESRL	US	FIM/NIM	OpenACC, F2C-ACC
NASA GSFC	US	GEOS-5	OpenACC (migration from CUDA-F
NCAR MMM	US	MPAS-A	OpenACC
NOAA GFDL	US	FV3	OpenACC
ECMWF	UK	IFS (Arpege)	Libs + OpenACC
STFC, MetOffice	UK	UM/GungHo	OpenACC
CSCS, MPI-M	CH, DE	ICON	DSL – dycore, OpenACC – physics
JAMSTEC, UT, RIKEN	JP	NICAM	OpenACC
(i) NCAR; (ii) SSEC	US	WRF-ARW	(i) OpenACC, (ii) CUDA
MCH, CSCS	СН	COSMO	DSL – dycore, OpenACC – physics
Bull	FR	HARMONIE	OpenACC

ASUCA

Regional



-			
Hybrid-F	[:] ortran,	OpenAC	C

Source: http://climatemodeling.science.energy.gov/sites/default/files/publications/acme-project-strategy-plan_0.pdf

US DOE Accelerator-Based Climate Model ACME

- ACME: Accelerated Climate Model for Energy
 - First fully accelerated climate model (GPU and MIC)
 - Consolidation of DOE ESM projects from 7 into 1
 - DOE Labs: Argonne, LANL, LBL, LLNL, ORNL, PNNL, Sandia

ACME a development branch of CESM from NCAR

- Atmosphere component CAM-SE (NCAR)
- Ocean component MPAS-O (LANL)
- Others: CICE (LANL), CLM (NCAR), SAM (CSU)
- Towards NH global atm 12 km, ocn 15 km, 80 years

Co-design project using US DOE LCF systems

First Report – 11 Jul 2014



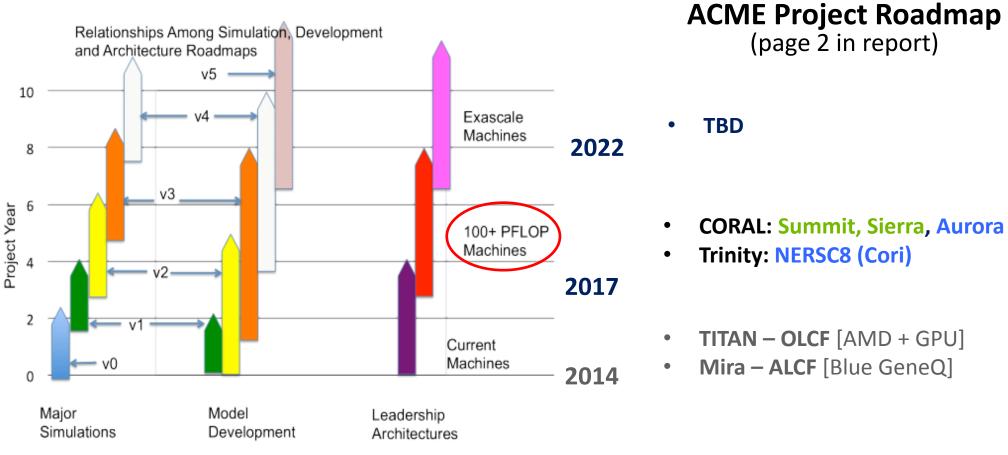
Accelerated Climate Modeling for Energy

Project Strategy and Initial Implementation Plan

Current Revision: July 11, 2014



Source: http://climatemodeling.science.energy.gov/sites/default/files/publications/acme-project-strategy-plan 0.pdf



US DOE Accelerator-Based Climate Model ACME



ICON ATM Climate Model and OpenACC

Current Status (May 2015)

PRACE 2IP extension has ended. So what is working?

- Dynamical core: I hr. R2B04 (4 GPUs) validates to I.E-I3.
- Implemented on GPU: solve_nh, diffusion, underlying routines, including mo_sync for communication
- Some advection schemes implemented (not in benchmark)
- Here: first publicly announced trunk NHDC benchmarks
- Actively porting 2-moment microphysics to OpenACC
- Radiation RRTMGP under discussion with Pincus, et al.

ETH Eldgendustuche Technische Hochschule Zürich Swiss Federal Institute of Technalogy Zurich



PASC15 Conference 01 Jun 15, ETH Zurich

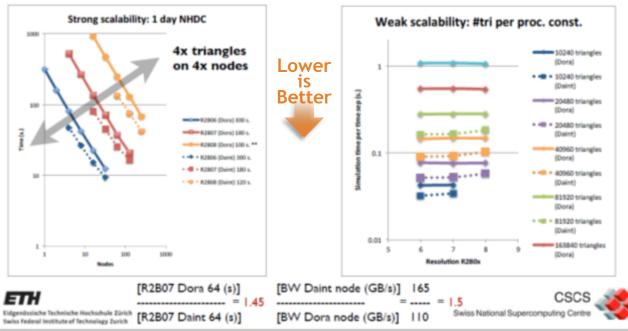
Using GPUs Productively for the ICON Climate Model -by Dr. Will Sawyer, CSCS

ICON Climate Model and OpenACC on GPUs



ICON Trunk NHDC on GPUs Results (New!)

Compare ICON Trunk Piz Dora (2x Haswell sockets) vs. Piz Daint nodes w/ K20x (both with Cray CCE)



PASC15 Conference 01 Jun 15, ETH Zurich

Using GPUs Productively for the ICON Climate Model -by Dr. Will Sawyer, CSCS

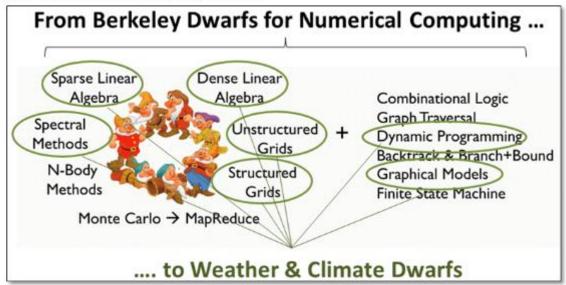
- Strong Scalability to 120 GPU nodes of Piz Daint
- Node comparisons of K20X vs. 2 x Haswell
- Non-hydrostatic dycore only, no nesting

ECMWF Project for Exascale Weather Prediction

Expectations towards Exascale: Weather and Climate Prediction – P. Bauer, ECMWF, EESI-2015

ESCAPE*, <u>Energy</u> efficient <u>SC</u>alable <u>Algorithms</u> for weather <u>Prediction</u> at <u>Exascale</u>:

- Next generation IFS numerical building blocks and compute intensive algorithms
- Compute/energy efficiency diagnostics
- New approaches and implementation on novel architectures
- Testing in operational configurations



*To be funded by EC H2020 framework, Future and Emerging Technologies – High-Performance Computing; Partners: **ECMWF**, Météo-France, RMI, DMI, Meteo Swiss, DWD, Loughborough U, PSNC, Bull, NVIDIA, Optalysys

EASCAPE HPC Goals:

- Standardized, highly optimized kernels on specialized hardware
- Overlap of communication and computation
- Compilers/standards
 supporting portability

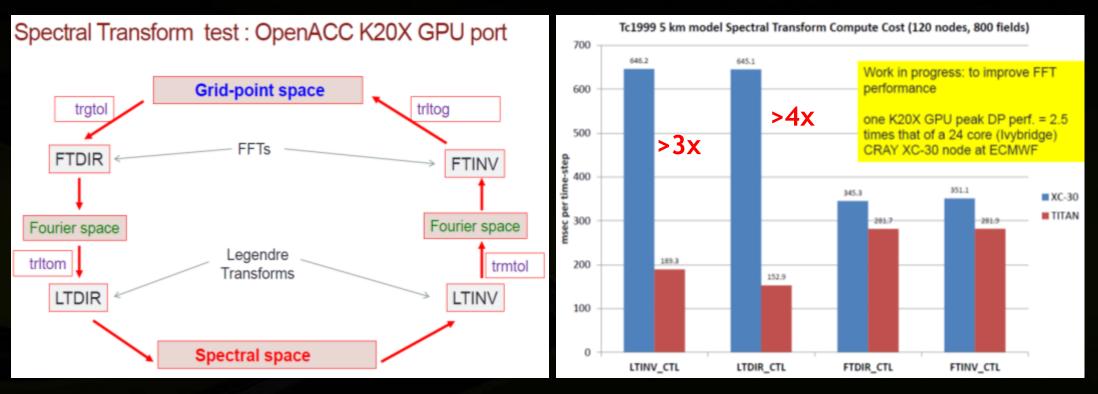
Project Approach:

 Co-design between domain scientists, computer scientists, and HPC vendors

ECMWF Initial IFS Investigation on Titan GPUs

Challenges of Getting ECMWF's Weather Forecast Model (IFS) to the Exascale

– G. Mozdzynski, ECMWF 16th HPC Workshop



Legendre Transform Kernels Observe >4x for Titan K20X vs. XC-30 24-core Ivy Bridge

NOAA NGGPS: NH Model Dycore Candidates (5)

Model	Organization	Numeric Method	Grid
NIM	NOAA/ESRL	Finite Volume	Icosahedral
MPAS	NCAR/LANL	Finite Volume	Icosahedral/Unstructured
NEPTUNE	Navy/NRL	Spectral Element	Cubed-Sphere with AMR
HIRAM/FV3	NOAA/GFDL	Finite Volume	Cubed-Sphere, nested
NMM-UJ	NOAA/EMC	Finite difference	Cubed-Sphere
GFS-NH	NOAA/EMC	Semi-Lagrangian/Spectral	Reduced Gaussian
IFS (RAPS13)	ECMWF	Semi-Lagrangian/Spectral	Reduced Gaussian

From: Next Generation HPC and Forecast Model Application Readiness at NCEP -by John Michalakes, NOAA NCEP; AMS, Phoenix, AZ, Jan 2015

Dycores FV3 & MPAS selected for Level-II evaluation – NVIDIA, **NOAA** investigating potential for GPUs **NOAA** evaluations under HPC program SENA – Software **Engineering for Novel** Architectures (2015)



GFDL Participation in GPU Hackathon Oct 2015



Mentors and content are contributed by recognized HPC leaders:

- USA: Oak Ridge National Laboratory, NCSA, Cray, NVIDIA, PGI
- Europe: CSCS, TU Dresden
- Japan: Tokyo Institute of Technology

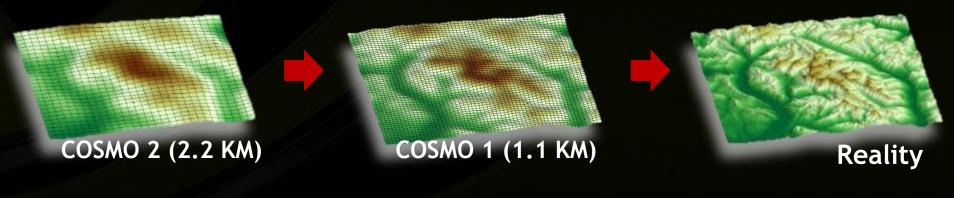
NOAA GFDL team led by Dr. Rusty Benson with NVIDIA and PGI members

COSMO Regional Model on GPUs



COSMO model fully implemented on GPUs by MeteoSwiss
 COSMO consortium approved GPU code for standard distribution

MeteoSwiss to deploy first-ever operational NWP on GPUs
 Successful daily test runs on GPUs since Dec 2014, operational in 2016



Source:

CSCS

Schweizerische Eidgenossensch Confédération suisse Confederazione Svizzera Confederaziun svizra "Increased Resolution = Quality Forecast"

WRF Progress Update



- Independent development projects of (I) CUDA and (II) OpenACC
 - I. CUDA through funded collaboration with SSEC <u>www.ssec.wisc.edu</u>



- SSEC lead Dr. Bormin Huang, NVIDIA CUDA Fellow: research.nvidia.com/users/bormin-huang
- Objective: Hybrid WRF benchmark capability starting 2H 2015

II. OpenACC directives through collaboration with NCAR MMM



Objective: NCAR GPU interest in Fortran version to host on distribution site

Project Status (II): NVIDIA-NCAR OpenACC WRF



- Objective to provide benchmark capability of hybrid CPU+GPU WRF 3.6.1
- NVIDIA ported 30+ routines to OpenACC for both dynamics and physics:
 - List provided on next page
 - Project to integrate OpenACC modules with full model WRF 3.6.1 release
 - Open source project with plans for NCAR hosting on WRF trunk distribution site
 - Objective to minimize code refactoring for scientists' readability and acceptance

NVIDIA - NCAR Project Success

- Several performance sensitive routines of dynamics and physics are completed
 - This includes advection routines for dynamics; expensive microphysics schemes
- Hybrid WRF performance using single socket CPU + GPU faster than CPU-only
 - Incremental improvements as more OpenACC code is developed for execution on GPU

WRF Modules Available in OpenACC



Project to implement OpenACC routines into full model WRF 3.6.1

- Several dynamics routines including all of advection
- Several physics schemes:
 - Microphysics Kessler, Morrison, Thompson
 - Radiation RRTM
 - Planetary boundary layer YSU, GWDO
 - Cumulus KFETA
 - Surface physics Noah

dyn_em/module_advect_em.OpenACC.F dyn_em/module_bc_em.OpenACC.F dyn_em/module_big_step_utilities_em.OpenACC.F dyn_em/module_diffusion_em.OpenACC.F dyn_em/module_em.OpenACC.F dyn_em/module_first_rk_step_part1.OpenACC.F dyn_em/module_first_rk_step_part2.OpenACC.F dyn_em/module_small_step_em.OpenACC.F dyn_em/module_stoch.OpenACC.F dyn_em/solve_em.OpenACC.F dyn_em/start_em.OpenACC.F frame/module_dm.OpenACC.F

frame/module_domain_extra.OpenACC.F
frame/module_domain.OpenACC.F
frame/module_domain_type.OpenACC.F
phys/module_bl_gwdo.OpenACC.F
phys/module_bl_ysu.OpenACC.F
phys/module_cu_kfeta.OpenACC.F
phys/module_microphysics_driver.OpenACC.F
phys/module_mp_kessler.OpenACC.F
phys/module_mp_morr_two_moment.OpenACC.F
phys/module_mp_thompson.OpenACC.F
phys/module_pbl_driver.OpenACC.F

phys/module_physics_addtendc.OpenACC.F
phys/module_physics_init.OpenACC.F
phys/module_ra_rrtm.OpenACC.F
phys/module_sf_noahlsm.OpenACC.F
phys/module_sf_sfclayrev.OpenACC.F
share/module_bc.OpenACC.F
share/wrf_bdyin.OpenACC.F

Project Status (I): NVIDIA-SSEC CUDA WRF



- Objective to provide Q3 benchmark capability of hybrid CPU+GPU WRF 3.6.1
- SSEC ported 20+ modules to CUDA across 5 physics types in WRF:
 - Cloud MP = 11; Radiation = 4; Surface Layer = 3; Planetary BL = 1; Cumulus = 1
 - Project to integrate CUDA modules into latest full model WRF 3.6.1
 - SSEC development began 2010, based on WRF 3.3/3.4 vs. latest release 3.6.1
 - Start with existing modules most common across target customer's input
 - Objective: speedups measured on individual modules within full model run

NVIDIA – SSEC Project Success

- Target modules achieve published GPU performance within full WRF model run
 - Final clean-up and performance studies underway, real benchmarks in 2H 2015
- TQI/SSEC to fund/port all modules to CUDA towards a full WRF model on GPUs
 - Focus on additional physics modules, and ongoing WRF-ARW dycore development

SSEC Speedups of WRF Physics Modules



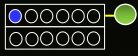
* Modules for initial NVIDIA-funded integration project

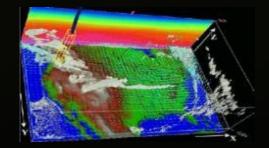
WRF Module	GPU Speedup (w-wo	I/O) Technical Paper Publication
Kessler MP	70x / 816x	J. Comp. & GeoSci., 52, 292-299, 2012
Purdue-Lin MP	156x / 692x	SPIE: doi:10.1117/12.901825
WSM 3-class MP	150x / 331x	
WSM 5-class MP *	202x / 350x	JSTARS, 5, 1256-1265, 2012
Eta MP	37x / 272x	SPIE: doi:10.1117/12.976908
WSM 6-class MP \star	165x / 216x	Submitted to J. Comp. & GeoSci.
Goddard GCE MP	348x / 361x	Accepted for publication in JSTARS
Thompson MP *	76x / 153x	
SBU 5-class MP	213x / 896x	JSTARS, 5, 625-633, 2012
WDM 5-class MP	147x / 206x	
WDM 6-class MP	150x / 206x	J. Atmo. Ocean. Tech., 30, 2896, 2013
RRTMG LW 🗶	123x / 127x	JSTARS, 7, 3660-3667, 2014
RRTMG SW *	202x / 207x	Submitted to J. Atmos. Ocean. Tech.
Goddard SW	92x / 134x	JSTARS, 5, 555-562, 2012
Dudhia SW \star	19x / 409x	
MYNN SL	6x / 113x	
TEMF SL	5x / 214x	
Thermal Diffusion LS	10x / 311x	Submitted to JSATRS
YSU PBL *	34x / 193x	Submitted to GMD

Hybrid WRF Customer Benchmark Capability Starting in 2H 2015

Hardware and Benchmark Case

CPU: Xeon Core-i7 3930K,1 core use;

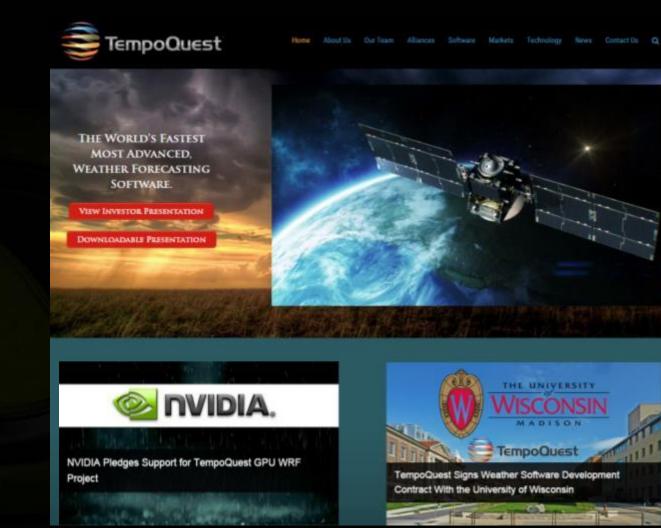




Benchmark: CONUS 12 km for 24 Oct 24; 433 x 308, 35 levels

TempoQuest USA Start-up to Commercialize WRF





TQI funds SSEC to complete all WRF modules to CUDA **Focus on ARW** dycore and additional physics

NVIDIA member of CUDA WRF project

Summary: Application Readiness for the Pre-Exascale Phase

NVIDIA observes strong ESM community interest in GPU acceleration

- Appeal of new technologies: Pascal, NVLink, more CPU platform choices
- NVIDIA applications engineering collaboration in several model projects

NVIDIA HPC technology behind the next-gen pre-exascale systems
 New GPU technologies combined with OpenPOWER for DOE CORAL

GPU progress for several models – we examined a few of these

- Climate models DOE ACME and MPI-M/CSCS ICON ATM
- NWP developments with ECMWF and ESCAPE, NOAA NGGPS, COSMO, WRF

Thank You

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