

# NVIDIA HPC Directions for Earth System Modeling

Stan Posey; [sposey@nvidia.com](mailto:sposey@nvidia.com); NVIDIA, Santa Clara, CA, USA

# **Agenda:** NVIDIA HPC Directions for ESM

- **NVIDIA HPC and GPU Update**
- **ES Model Progress on GPUs**
- **GPU Technology Roadmap**

# NVIDIA - Core Technologies and Products



Company Revenue of ~\$5B USD; ~8,500 Employees; HPC Growing > 35% CAGR

## GPU



GeForce<sup>®</sup>  
Quadro<sup>®</sup>, Tesla<sup>®</sup>

## Mobile



Tegra<sup>®</sup>

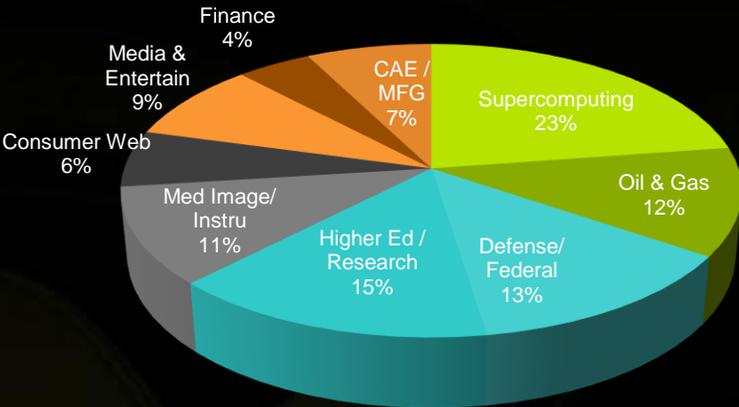
## Cloud



GRID

# GPUs Mainstream Across Diverse HPC Markets

FY14 Segments



Oil & Gas	Higher Ed	Government	Supercomputing	Finance	Web 2.0

World's Top 3 Servers are GPU-Accelerated



R720



DL380

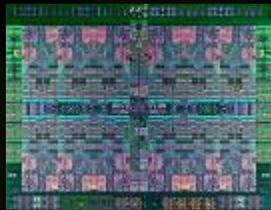


**lenovo** x3650

# IBM Power + NVIDIA GPU Accelerated HPC

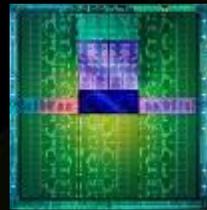
## Next-Gen IBM Supercomputers and Enterprise Servers

Long term roadmap integration



POWER CPU

+



Tesla GPU

## OpenPOWER Foundation

Open ecosystem built on Power Architecture



& 30+ more...

First GPU-Accelerated POWER-Based Systems Available in Oct 2014

# Cray + NVIDIA GPU Accelerated HPC

- Cray and NVIDIA Collaboration on Large Systems
  - **TITAN** – Oak Ridge National Laboratory, **#2 Top 500**
  - **Gaea** – NOAA (managed on-site at Oak Ridge)
  - **Piz Daint** – Swiss Supercomputing Center, **#6 Top 500**
  - **Blue Waters** – National Center for Scientific Applications



TITAN - ORNL



Piz Daint - CSCS



## News Release

### Cray Launches New High Density Cluster Packed With NVIDIA GPU Accelerators

SEATTLE, WA -- (Marketwired) -- 08/26/14 -- Global supercomputer leader Cray Inc. (NASDAQ: CRAY) today announced the launch of the Cray CS-Storm -- a high-density accelerator compute system based on the Cray® CS300™ cluster supercomputer. Featuring up to eight NVIDIA® Tesla® GPU accelerators and a peak performance of more than 11 teraflops per node, the Cray CS-Storm system is one of the most powerful single-node cluster architectures available today.

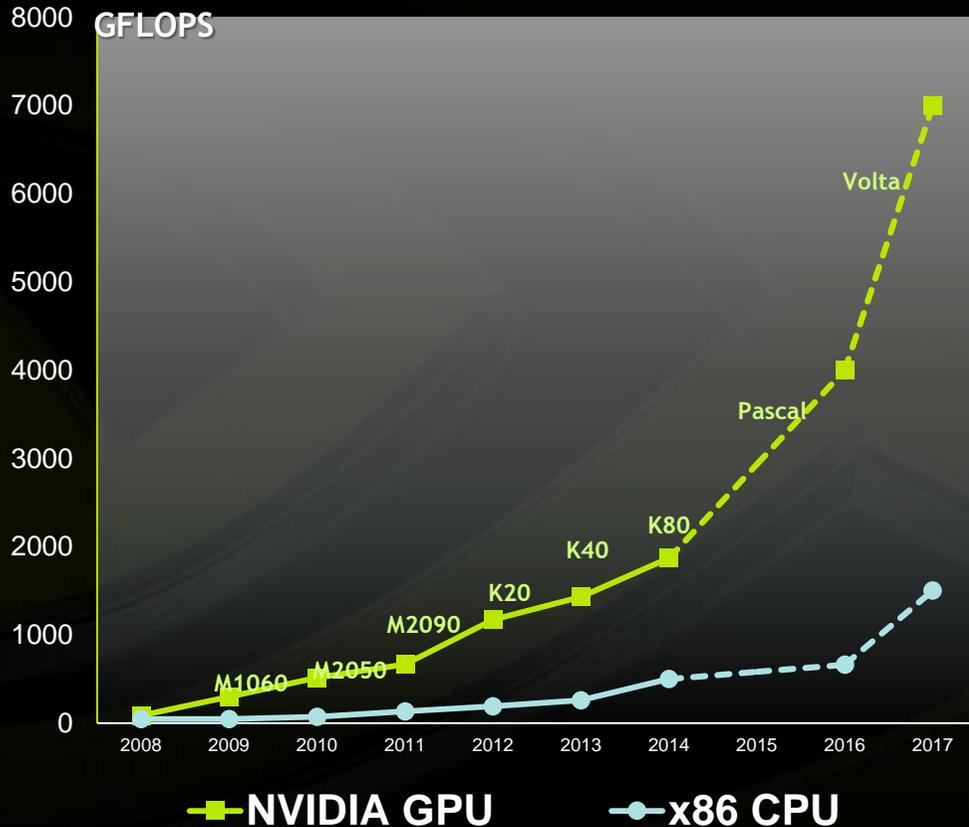
16 Aug 2014

### Cray Launches High Density CS-Storm with NVIDIA K40 GPUs

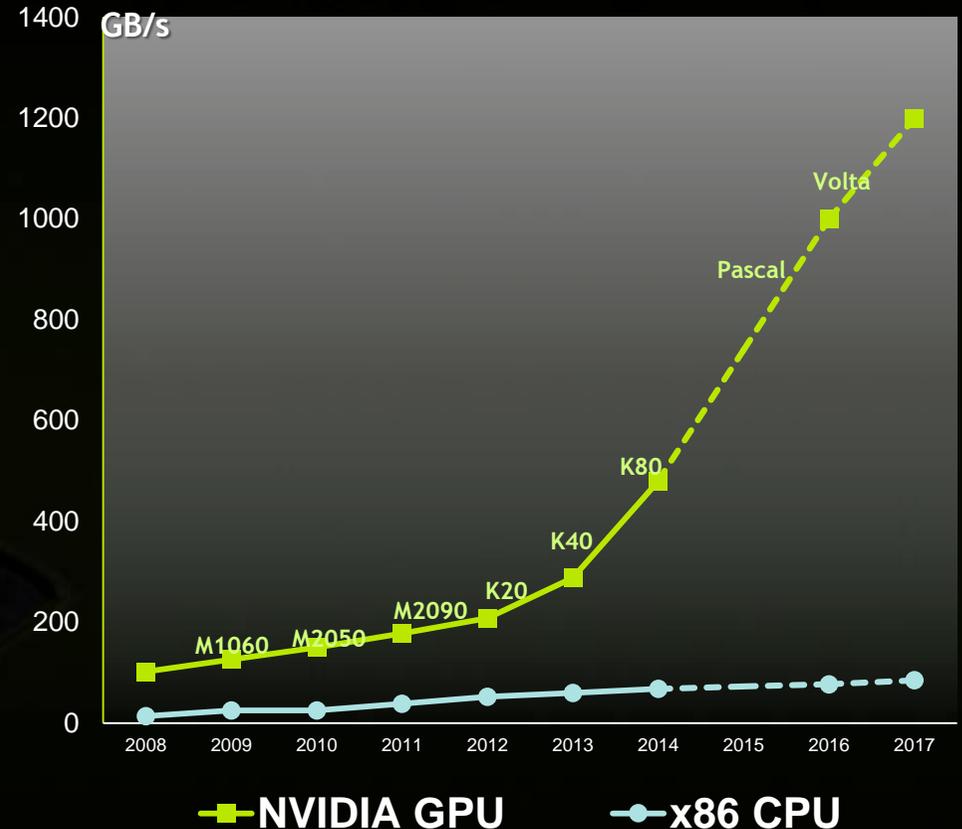
- Up to 8 x K40 per node
- Capable of 1 PF per 4 Racks

# GPU Motivation (I): Performance Trends

## Peak Double Precision FLOPS



## Peak Memory Bandwidth





# GPU Motivation (II): Energy Efficient HPC

Top500 Rank	TFLOPS/s	Site	
1	33,862.7	National Super Computer Centre Guangzhou	
2	17,590.0	Oak Ridge National Lab <b>#1 USA</b>	
3	17,173.2	DOE, United States	
4	10,510.0	RIKEN Advanced Institute for Computational Science	
5	8,586.6	Argonne National Lab	
6	6,271.0	Swiss National Supercomputing Centre (CSCS) <b>#1 Europe</b>	
7	5,168.1	University of Texas	
8	5,008.9	Forschungszentrum Juelich	
9	4,293.3	DOE, United States	
10	3,143.5	Government	

Green500 Rank	MFLOPS/W	Site	
1	4,389.82	GSIC Center, Tokyo Tech <b>KFC</b>	
2	3,631.70	Cambridge University	
3	3,517.84	University of Tsukuba	
4	3,459.46	SURFsara	
5	3,185.91	Swiss National Supercomputing (CSCS)	
6	3,131.06	ROMEO HPC Center	
7	3,019.72	CSIRO	
8	2,951.95	GSIC Center, Tokyo Tech <b>2.5</b>	
9	2,813.14	Eni	
10	2,629.10	(Financial Institution)	
16	2,495.12	Mississippi State (top non-NVIDIA) <b>Intel Phi</b>	
59	1,226.60	ICHEC (top X86 cluster)	

# GPU Motivation (III): Model Trends in ESM

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



Source: Project Athena – <http://www.wxmaps.org/athena/home/>

- Increase ensemble use and ensemble members to manage uncertainty



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

Accelerator technology identified as a cost-effective and practical approach to future computational challenges

# Hardware Trends: NWP/Climate HPC Centers



Motivation for x86 Migration Includes Preparation for Future Accelerator Deployment

Operational NWP

Organization	Location	Models	Previous/Current Operational HPC	Current/Next Operational HPC
ECMWF	Reading, UK	IFS	IBM Power	Cray XC30 – x86
Met Office	Exeter, UK	UM	IBM Power	Cray XC30 – x86
DWD	Offenbach, DE	GME, COSMO, ICON	NEC SX-9	Cray XC30 - x86
MF	Toulouse, FR	ALADIN, AROME	NEC SX-9	Bull - x86
NOAA/NCEP	<i>Various</i> , US	GFS, WRF, FIM, NIM	IBM Power	IBM iDataPlex - x86

Research

NCAR	Boulder, US	CESM, WRF, MPAS	IBM Power	IBM iDataPlex - x86
DKRZ/MPI-M	Hamburg, DE	MPI-ESM	IBM Power	Bull - x86

# NVIDIA GPU Technology and ESM Strategy

## Technology

- **Development of GPUs as a co-processing accelerator for CPUs**



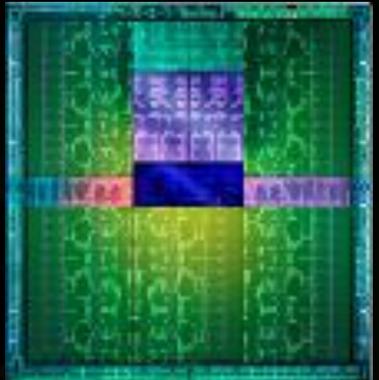
## Strategy

- **Investments and alliances to develop Fortran-based programming environment**
- **Collaborations that provides applications engineering support in 16 model projects**
- **GPU integration and support on large systems with vendors (Cray, IBM, Bull, etc.)**

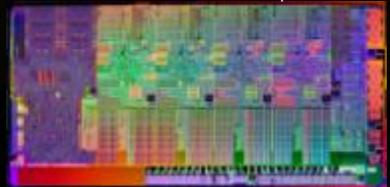
# New CPU Platforms Available During 2014



## Tesla K40 (Kepler)



PCIe - 16 GB/s



X86 | ARM64 | Power8

# Tesla GPU Progress Since 15<sup>th</sup> HPC Workshop



	ECMWF 15 <sup>th</sup> Workshop <b>M2075</b>	<b>K20X</b>	<b>K40</b>	15 <sup>th</sup> / 16 <sup>th</sup> Progress
Peak SP Peak SGEMM	1.03 TF	3.93 TF 2.95 TF	4.29 TF 3.22 TF	~ 4x
Peak DP Peak DGEMM	.515 TF	1.31 TF 1.22 TF	1.43 TF 1.33 TF	~3x
Memory size	6 GB	6 GB	<b>12 GB</b>	<b>2x</b>
Mem BW (ECC off)	150 GB/s	250 GB/s	<b>288 GB/s</b>	<b>~2x</b>
Memory Clock		2.6 GHz	3.0 GHz	
PCIe Gen	Gen 2	Gen 2	<b>Gen 3</b>	<b>~2x</b>
# of Cores	448	2688	2880	~5x
Core Clock		732 MHz	Base: 745 MHz Boost: 875 Mhz	
Total Board Power	<b>235W</b>	<b>235W</b>	<b>235W</b>	<b>Same</b>

# Agenda: NVIDIA HPC Directions for ESM

- NVIDIA HPC and GPU Update
- **ES Model Progress on GPUs**
- GPU Technology Roadmap

# Tesla K40 Results from Multi-Core 4 Workshop



NCAR  
UCAR



## 2014 Heterogeneous Multi-Core 4 Workshop

September 17-18, 2014 at the National Center for Atmospheric Research in Boulder, Colorado

<https://www2.cisl.ucar.edu/heterogeneous-multi-core-4-workshop/2014>

### 1. Modernizing Legacy Codes

- Youngsung Kim, NCAR CISL; Source: [https://www2.cisl.ucar.edu/sites/default/files/youngsung\\_1.pdf](https://www2.cisl.ucar.edu/sites/default/files/youngsung_1.pdf)

### 2. Directive-Based Parallelization of the NIM

- Mark Govett, NOAA ESRL; Source: [https://www2.cisl.ucar.edu/sites/default/files/govett\\_3.pdf](https://www2.cisl.ucar.edu/sites/default/files/govett_3.pdf)

### 3. Optimizing Weather Model Radiative Transfer Physics for the Many Integrated Core and GPGPU Architectures

- John Michalakes, NOAA NCEP; Source: [https://www2.cisl.ucar.edu/sites/default/files/michalakes\\_1.pdf](https://www2.cisl.ucar.edu/sites/default/files/michalakes_1.pdf)

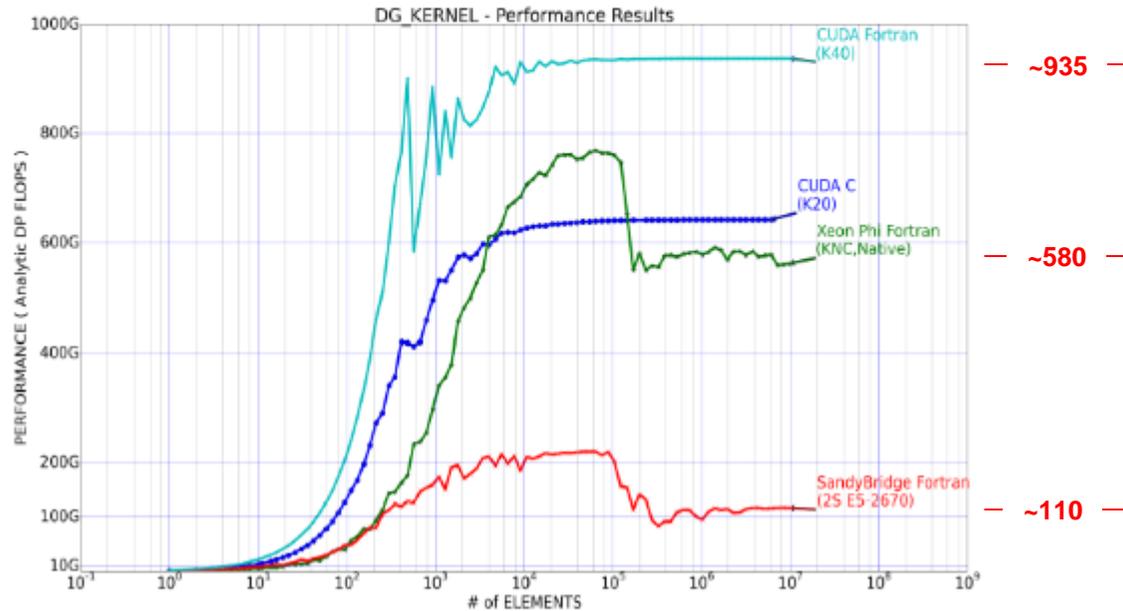
### 4. CUDA WRF Development Project at SSEC (presented at NVIDIA roadmap review)

- Jarno Mielikainen, SSEC UW-Madison; Source: contact Stan Posey, [sposey@nvidia.com](mailto:sposey@nvidia.com) for full presentation

# 1. Tesla K40 Results: NCAR-CISL DG Kernels

## We've learned some about

- how to get performance from new processors



## SUMMARY

### K40 Speed-ups

Sandy Bridge 8.5x

Xeon Phi (Native) 1.6x

#### NOTES:

- Results for Number of Elements =  $10^7$
- K40 results from optimized CUDA Fortran

# 2. Tesla K40 Results: NOAA-ESRL and NIM

## NIM Dynamics: Single Node Performance

Numeric values represent node run-times for each configuration



### Parallelization and Performance

- Single source code (NIM rev 2724)
- Directive-based parallelization
  - OpenMP CPU, MIC
  - F2C-ACC GPU
  - SMS MPI
  - OpenACC GPU

### System / Node configurations

- NVIDIA PSG Cluster
  - IB20: Intel IvyBridge, 20 cores, 3.0 GHz (Intel E5-2690 v2)
  - GPU: Kepler K40 2880 cores, 745 MHz, 12GB memory
- Intel Endeavor Cluster
  - IB24: Intel IvyBridge 24 cores, 2.70 GHz (Intel E5-2697 v2)
  - MIC: KNC 7120 61 cores, 1.238 GHz, 16 GB memory

<http://www.esrl.noaa.gov/gsd/ab/ac/NIM-Performance.html>

## SUMMARY

### K40 Speed-ups

2 x Ivy Bridge 1.3x

Xeon Phi 1.3x

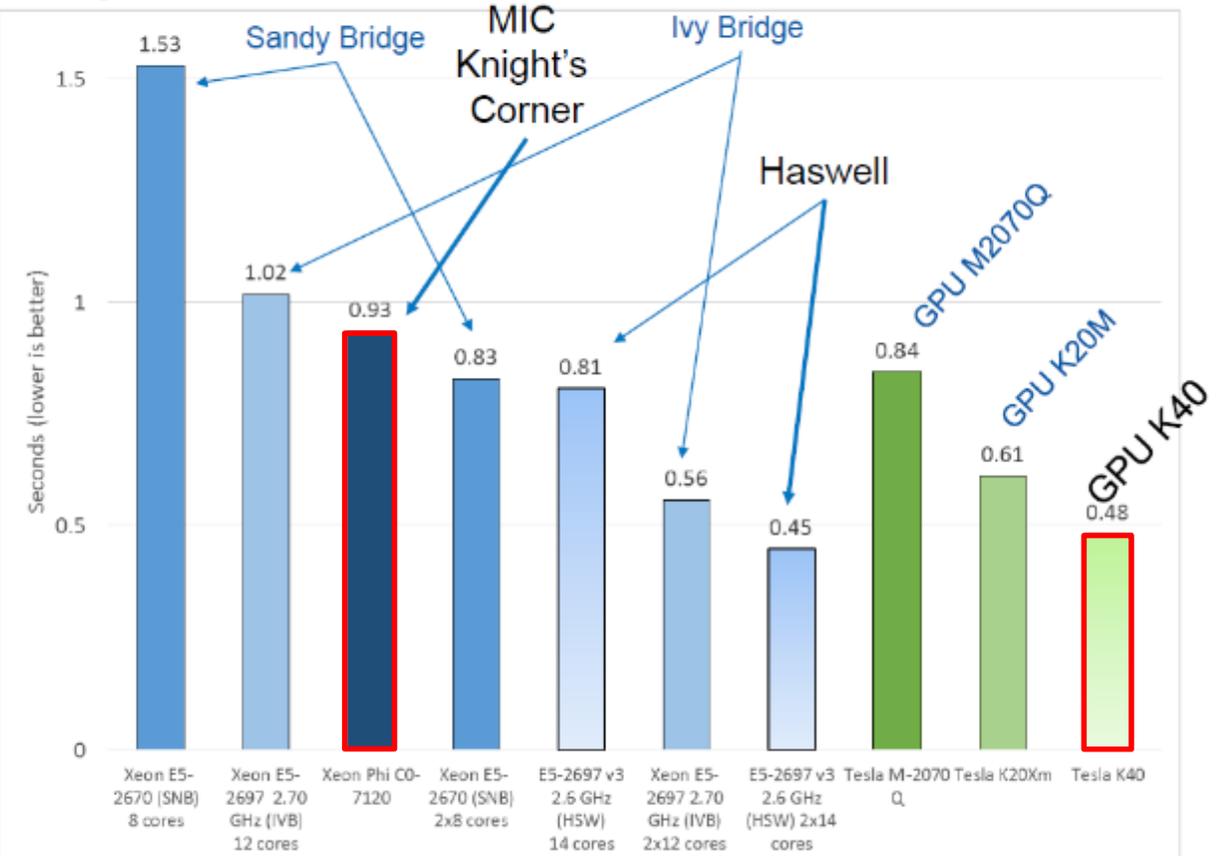
### NOTES:

- Results for standalone CPUs and accelerators
- K40 results from use of F2C-ACC

# 3. Tesla K40 Results: NOAA-NCEP and RRTMG



## Comparison to GPU Performance



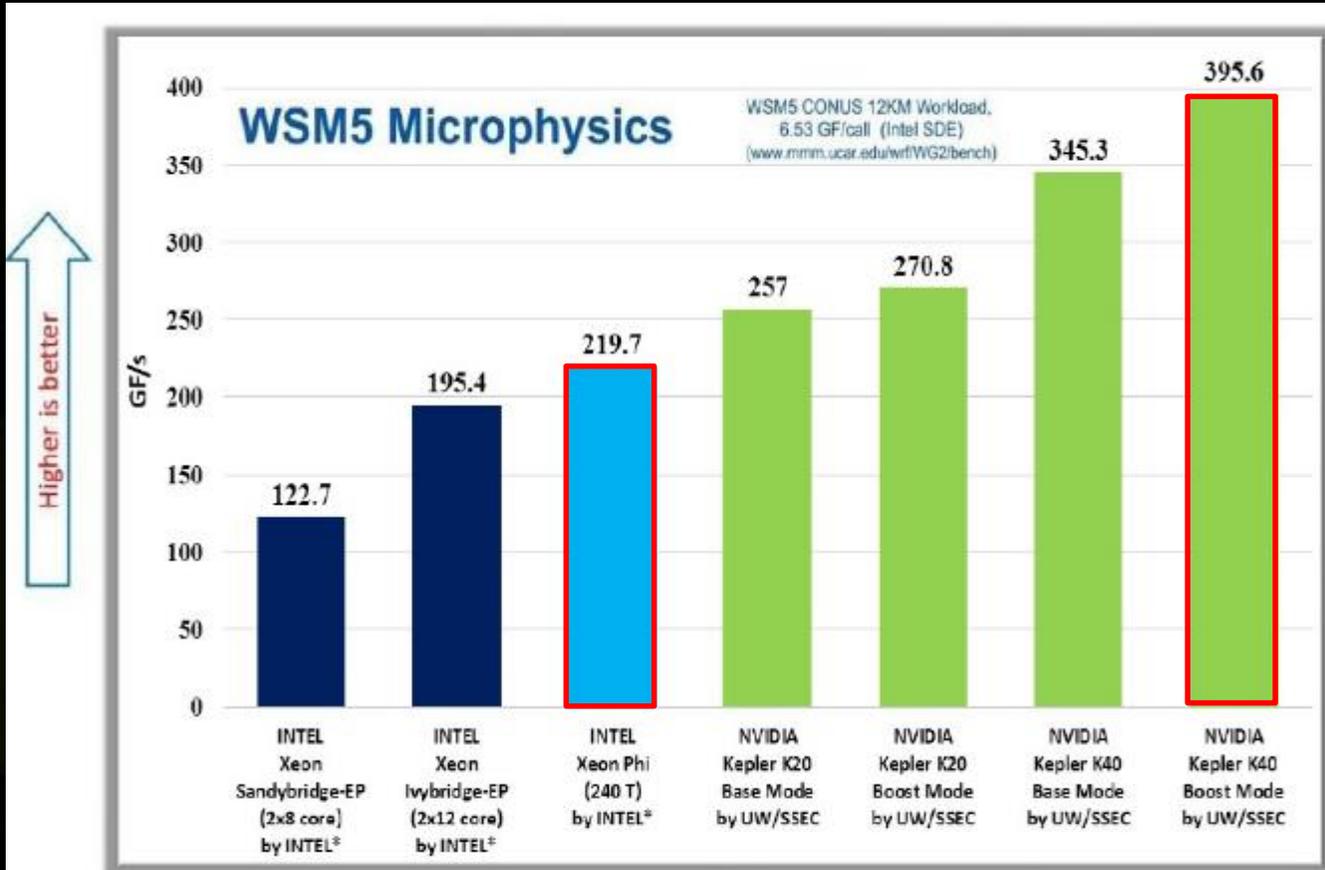
### SUMMARY

#### K40 Speed-ups

2 x Sandy Bridge	1.7x
2 x Ivy Bridge	1.2x
2 x Haswell	0.9x
1 x Haswell	1.7x
Xeon Phi (Native)	1.9x



# 4. Tesla K40 Results: SSEC and WRF WSM5



\* Code Restructuring to Improve Performance in WRF Model Physics on Intel Xeon Phi. J. Michalakes. Workshop on Programming Weather, Climate and Earth System Models on Heterogeneous Multi-core Platforms, Boulder, Colorado, Sept. 19-20, 2013. ([http://data1.gfdl.noaa.gov/multi-core/presentations/michalakes\\_5.pdf](http://data1.gfdl.noaa.gov/multi-core/presentations/michalakes_5.pdf))

## SUMMARY

### K40 Speed-ups

2 x Sandy Bridge	3.2x
2 x Ivy Bridge	2.0x
Xeon Phi	1.8x

# Tesla K40 Results from Multi-Core 4 Workshop



## 2014 Heterogeneous Multi-Core 4 Workshop

September 17-18, 2014 at the National Center for Atmospheric Research in Boulder, Colorado  
<https://www2.cisl.ucar.edu/heterogeneous-multi-core-4-workshop/2014>

## Summary

- **Tesla K40 GPU the faster accelerator for each of the comparisons provided**

Workshop Study	NCAR CISL CESM DG Kernels	NOAA ESRL NIM	NOAA NCEP RRTMG	SSEC WRF WSM5
K40 / Phi Speed-up	1.6x	1.3x	1.9x	1.8x

- **IMPORTANT:** all results are based on a CUDA programming environment
  - CUDA may not be suitable for production-level development/deployment
  - Most operational models require Fortran – therefore an **OpenACC** approach

# OpenACC Vital to ESM Production use of GPUs

## NVIDIA Investments in OpenACC Standard

- NVIDIA acquisition of PGI, both OpenACC members; Ongoing Cray collaborations
- Support on important contributions from end-user members NOAA ESRL, CSCS/MCH, etc.
- Support/training to OpenACC members who have NWP/Climate GPU developments



## OpenACC Workshops for the ESM Community

- Mar 2014: **GTC OpenACC Roundtable for NWP and Climate Modeling** (10 Models Reviewed)
- Sep 2014: **NVIDIA Three Years HPC Roadmap Review for ESM** (1/2 day OpenACC Focus)
- Oct 2014: **DOE Oak Ridge Lab GPU and OpenACC HACK-A-THON** (HYCOM, CICE, MPAS-O?)

<https://www.olcf.ornl.gov/training-event/hackathon-openacc2014/>

## Examples of OpenACC ESM Implementation

- Published OpenACC results on model success: **COSMO, ICON, NICAM, NIM, NEMO**

# NVIDIA HPC Roadmap Review for ESM –Sep 2014

19 Sep 14, Boulder, CO, USA – Following the Multi-Core 4 Workshop

**Agenda:** Welcome and NVIDIA HPC Strategy Update for ESM Community

**Roadmap of 3 Years Outlook for GPU Hardware and Software**

- Dale Southard, Chief HPC Architect, NVIDIA Office of the CTO

**Invited Talk on CUDA WRF Development Project at SSEC**

- Dr. Jarno Mielikainen, Senior Staff Scientist, [SSEC UW-Madison](#)

**OpenACC Features and Fortran Programming Considerations**

- Jeff Larkin, Sr. HPC Engineer, NVIDIA Developer Technology Group

**Cray Roadmap for OpenACC 2.0 and Beyond**

- Eric Dolven, Cray

**PGI Roadmap for OpenACC 2.0 and Beyond**

- Dave Norton, Sr. HPC Applications Engineer, PGI

**OpenACC  
Features and  
Roadmap 1/2  
Day Focus**

**Delegates:** USA – **NCAR** (CISL, MMM); **NOAA** (ESRL, GFDL, NCEP); **NASA GSFC**; **DOE** (ORNL, ANL, PNNL, SNL)  
INTL – **Met Office** (UK), **STFC** Daresbury (UK), **KISTI** (KR)

- Motivation to identify critical and common OpenACC requests for international selection of 10 models

<b>Model</b>	<b>Representatives</b>
1. ASUCA	<i>Takashi Shimokawabe, TiTech; Michel Müller, RIKEN</i>
2. CAM-SE	<i>Jeff Larkin, NVIDIA US; Matt Norman, ORNL</i>
3. COSMO	<i>Peter Messmer, NVIDIA CH; Claudio Gheller, Will Sawyer, CSCS</i>
4. FIM/NIM	<i>Mark Govett, NOAA</i>
5. HARMONIE	<i>JC Desplat, Enda O'Brien, ICHEC</i>
6. ICON	<i>Peter Messmer, NVIDIA CH; Claudio Gheller, Will Sawyer, CSCS</i>
7. NEMO	<i>Jeremy Appleyard, NVIDIA UK</i>
8. NICAM	<i>Akira Naruse, NVIDIA JP; Hisashi Yashiro, RIKEN</i>
9. WRF	<i>Carl Ponder, NVIDIA US</i>
10. COAMPS	<i>Dave Norton, PGI; Gopal Patnaik, US NRL</i>

# Results of GTC OpenACC Roundtable (I)



## OpenACC Feature Request

- Support for derived types with member arrays in data clauses
- Deep copy support:
  - Arrays of derived type with member arrays of derived type with member arrays, etc.; **CAM-SE, COSMO, ICON, HARMONIE**
  - Deep and shallow copy for nested derived types, selective deep copy; **ICON, HARMONIE**
- Minimize code restructuring such as inner-outer loop reordering; **CAM-SE, others**
- Want consistent experiences across vendor implementations:
  - Perhaps more strict specification so different implementations have less freedom to interpret; **NIM**
  - User desires to write program once that will port to different systems/compilers

## PGI Response

- Initial support in 14.4 released Apr 2014
- **Not supported, plans not yet announced**
- In development, initial support in 14.7 (Jul)
- No response, but close collaboration with OpenACC member alliance on specifications

# Results of GTC OpenACC Roundtable (II)



## OpenACC Feature Request

- Allow allocation of noncontiguous array sections such as matrix interior; **HARMONIE**
- Allow unallocated arrays in data clauses; **HARMONIE**
- Bitwise consistency between CPU and GPU; **ICON**
- Expose pinned memory; **NIM, NICAM**
- Expose shared memory; **WRF**
- Reorder array dimensions for CPU vs. GPU; **ASUKA, others**
- Full procedure support with no restrictions, and no specification required on subroutine definition; **COAMPS**
- Expose managed memory; **NEMO**
- CUDA Aware MPI or OpenACC aware MPI

## PGI Response

- **Not supported, plans not yet announced**
- In development, initial support in 14.7 (Jul)
- Investigating for support, no release plan
- No plans announced, but under consideration
- No plans announced, but under consideration
- **Not supported, plans not yet announced**
- **Not supported, plans not yet announced**
- Investigating with CUDA 6, support in 14.7
- No plans announced, but under consideration

# COSMO



## Towards GPU-accelerated Operational Weather Forecasting

- Oliver Fuhrer (MeteoSwiss), NVIDIA GTC 2013, **Mar 2013**

Source: <http://on-demand.gputechconf.com/gtc/2013/presentations/S3417-GPU-Accelerated-Operational-Weather-Forecasting.pdf>

## Implementation of COSMO on Accelerators

- Oliver Fuhrer (MeteoSwiss), ECMWF Scalability Workshop, **Apr 2014**

Source: <http://old.ecmwf.int/newsevents/meetings/workshops/2014/Scalability/>

### Piz Daint System

[http://www.cscs.ch/piz\\_daint/](http://www.cscs.ch/piz_daint/)

- Piz Daint consists of 5272 compute nodes with 169 TB of total system memory
- Each node contains 1 x Intel Xeon E5-2670 CPU and 1 x NVIDIA K20X GPU
- COSMO operational tests up to 1000's of nodes on Piz Daint Cray XC30

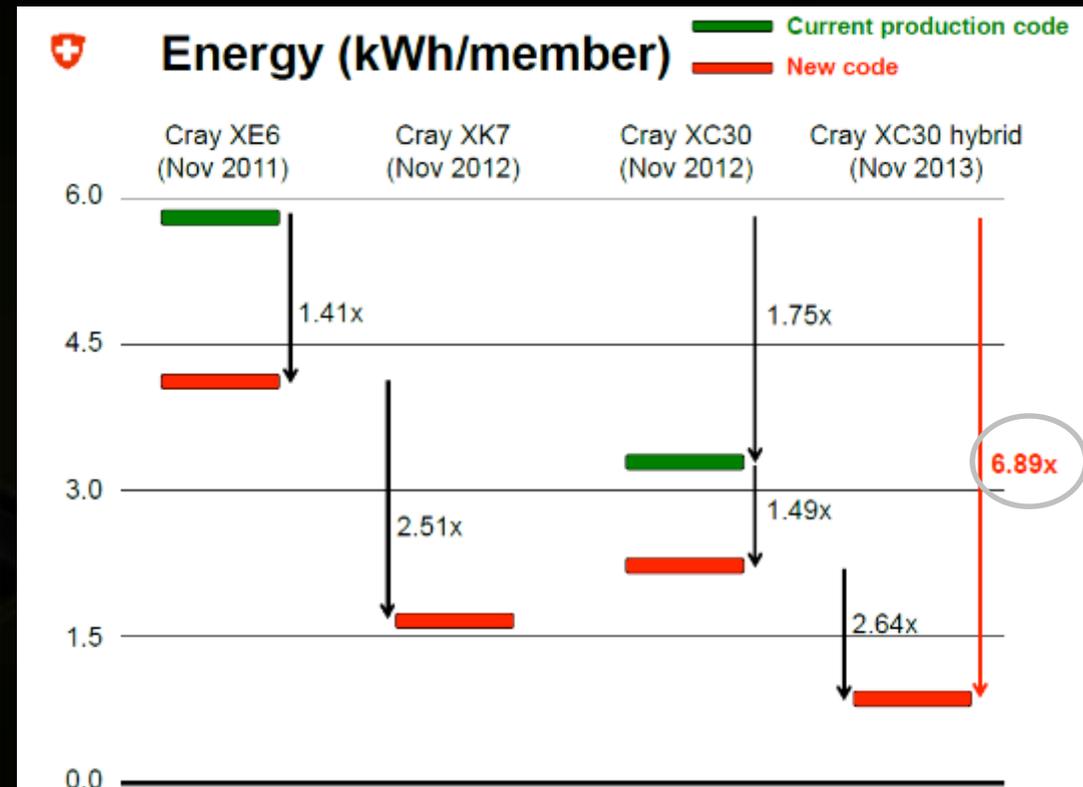
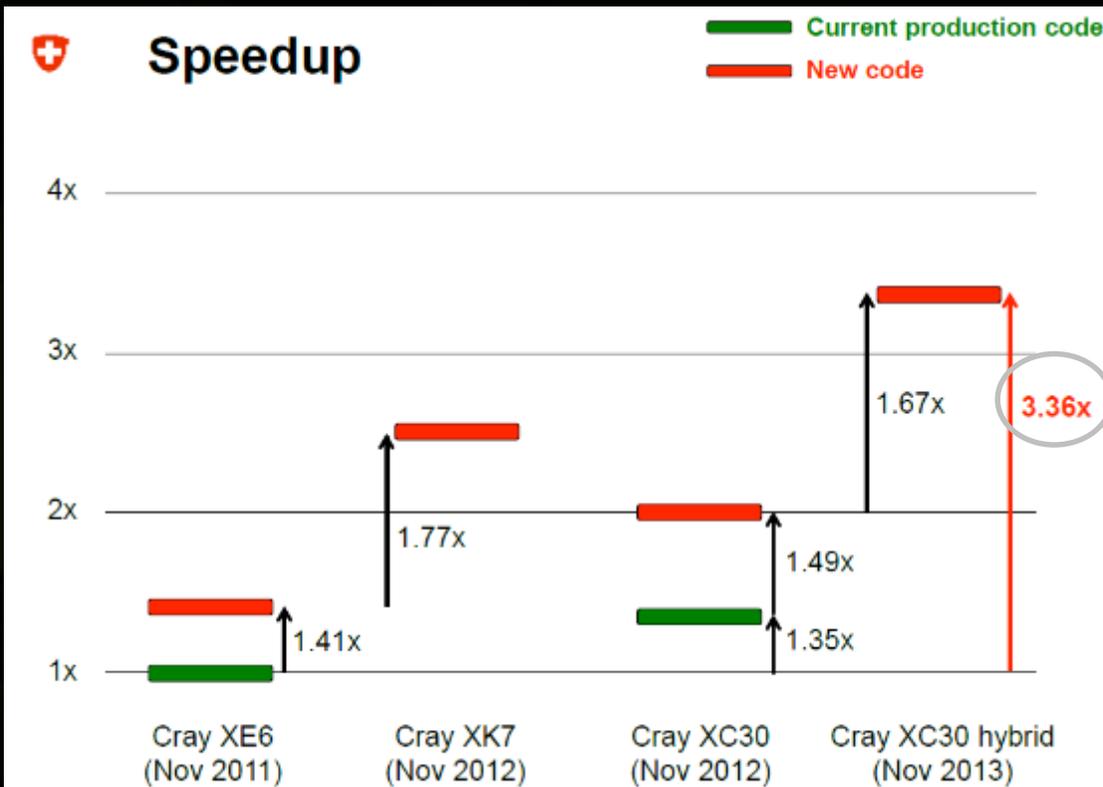


# COSMO Results from ECMWF Scalability Workshop

## Implementation of COSMO on Accelerators

-by Dr. Oliver Fuhrer, MeteoSwiss; ECMWF Scalability Workshop, Apr 2014

**CUDA-based DSL "STELLA" for dynamics + OpenACC for physics and data assimilation**



# NEMO

## Accelerating NEMO with OpenACC

- Maxim Milakov (NVIDIA), NVIDIA GTC 2013, **Mar 2013**

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

## NEMO on GPU-based Heterogeneous Architectures: a Case Study Using OpenACC

- Jeremy Appleyard (NVIDIA), NEMO UGM, **Jul 2014**

# NEMO Performance with OpenACC and GPUs



## NEMO Model

<http://www.nemo-ocean.eu/>

- Nucleus for European Modelling of the Ocean global and regional OGCM
- Primary developers CNRS, Mercato-Ocean, UKMO, NERC, CMCC, INGV
- OCN component for 5 of 7 Earth system models in the ENES <http://enes.org>
- European consortium of 40 projects, 400 users, and ~50 publications/year

**NEMO**



## Configurations

- **GYRE50:** Idealized double gyres, 1/4° horizontal resolution, 31 vertical layers
- **ORCA025:** Global high resolution, 1/4° horizontal resolution, 75 vertical layers



## NVIDIA “PSG” Cluster

<http://psgcluster.nvidia.com/trac>

- PSG consists of 30 compute nodes of mixed type, each 128 GB of system memory
- This study: Each node 2 x Intel Xeon Ivy Bridge CPUs and 6 x NVIDIA K40 GPUs
- NEMO tests on 8 nodes using 20 of 20 cores per node, and 2 of 6 GPUs per node



# NEMO Coupling to European Climate Models

- NEMO critical for European climate models: ocean component for 5 of 7 modeling groups\*



Country	name of model (CMIP5)	Atmosphere	Ocean	Sea Ice	Coupler	Land Surface *Vegetation	Atmospheric Chemistry	Ocean Bio-geochemistry
Consortium	EC-EARTH	IFS	NEMO	LIM	OASIS	HTESSEL	TM5	
France	IPSLCM5	LMDz	NEMO	LIM	OASIS	ORCHIDEE	INCA	PISCES
France	CNRM-Cerfacs	ARPEGE	NEMO	GELATO	OASIS	SURFEX		
Germany	MPI-ESM	ECHAM5	MPIOM	MPIOM	OASIS	JSBACH*	HAM	HAMOCC
Italy	C-ESM	ECHAM5	NEMO	LIM	OASIS	SILVA		PELAGOS
UK	HadGEM2	UM	UM	CICE	OASIS	TRIFFID*	UKCA	diat-HADOCC
Norway	NorESM	NCAR	MICOM	CICE	CPL7	CLM	Chemistry	HAMOCC

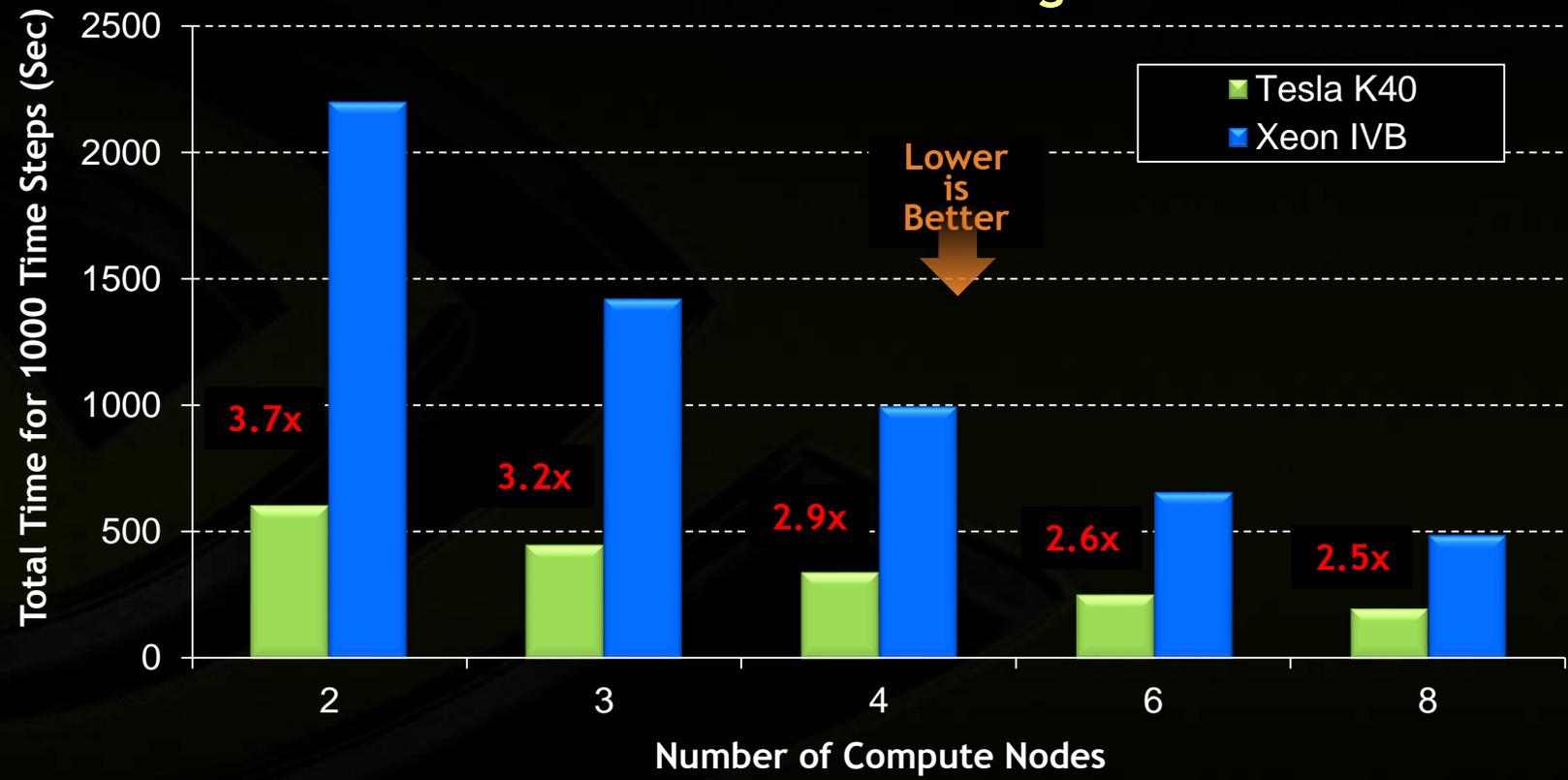
EC-Earth Con Netherlands, Sweden, Ireland, Denmark, Spain, Portugal, Italy, Belgium

\* UKMO has announced NEMO as the ocean component model for HadGEM3

# NEMO Performance with OpenACC and GPUs



## NEMO GYRE 1/4° Configuration



**PSG node utilization:**  
2 x IVB + 2 x K40

Without using GPUs

Use of GPUs

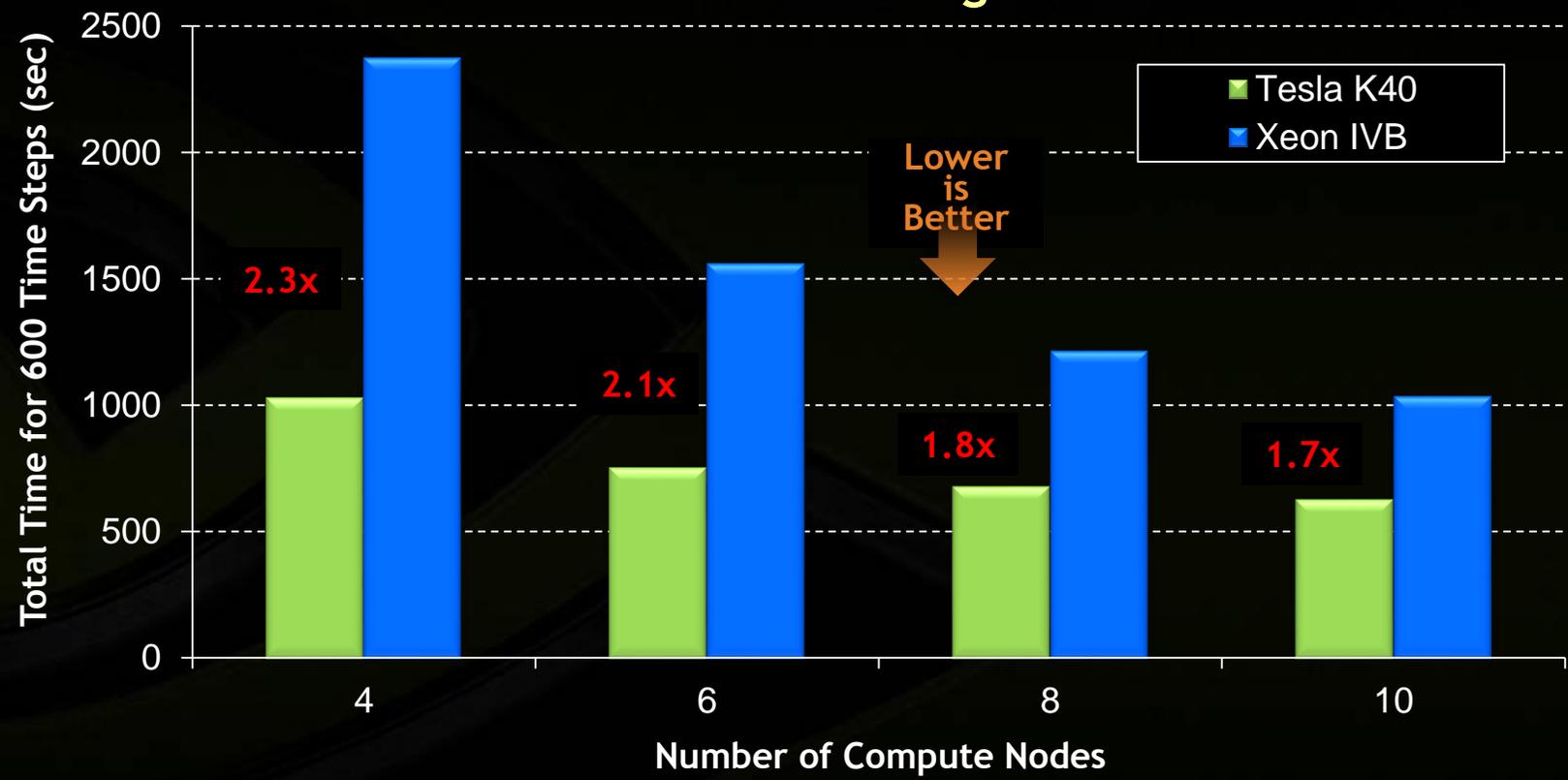
**GYRE settings:**

- Output every 5 days
- Time steps = 1000
- NEMO release 3.5

# NEMO and GPU Performance with OpenACC



## ORCA025 Configuration



**Node utilization:**  
2 x IVB + 2 x K40

Without using GPUs

Use of GPUs

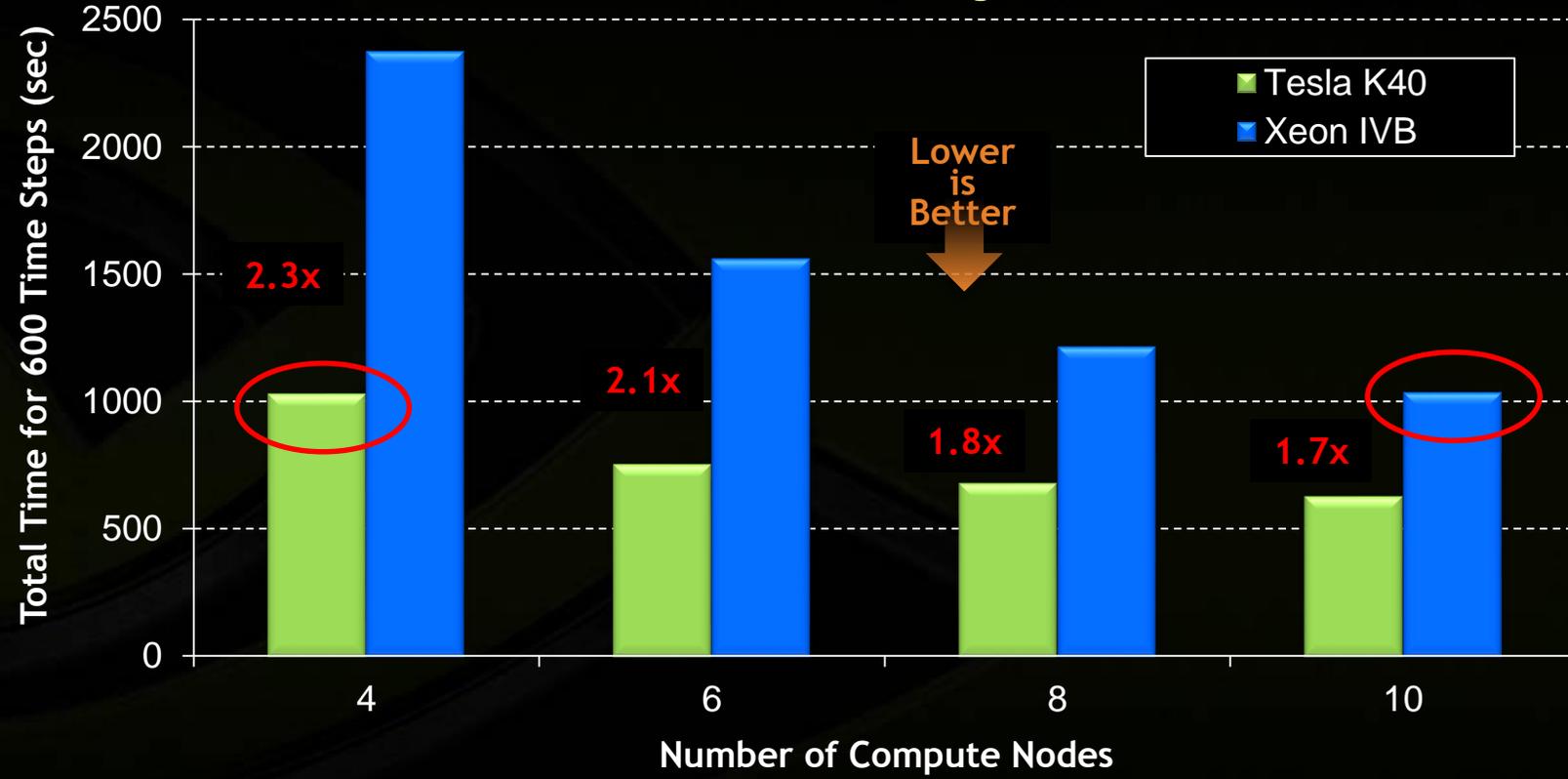
**ORCA025 settings:**

- Output every 5 days
- Total run: 10 days
- Time steps: 600
- NEMO 3.5

# NEMO and GPU Performance with OpenACC

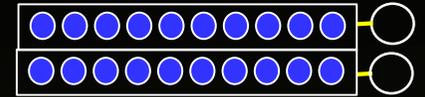


## ORCA025 Configuration

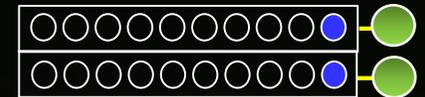


**Node utilization:**  
2 x IVB + 2 x K40

Without using GPUs



Use of GPUs



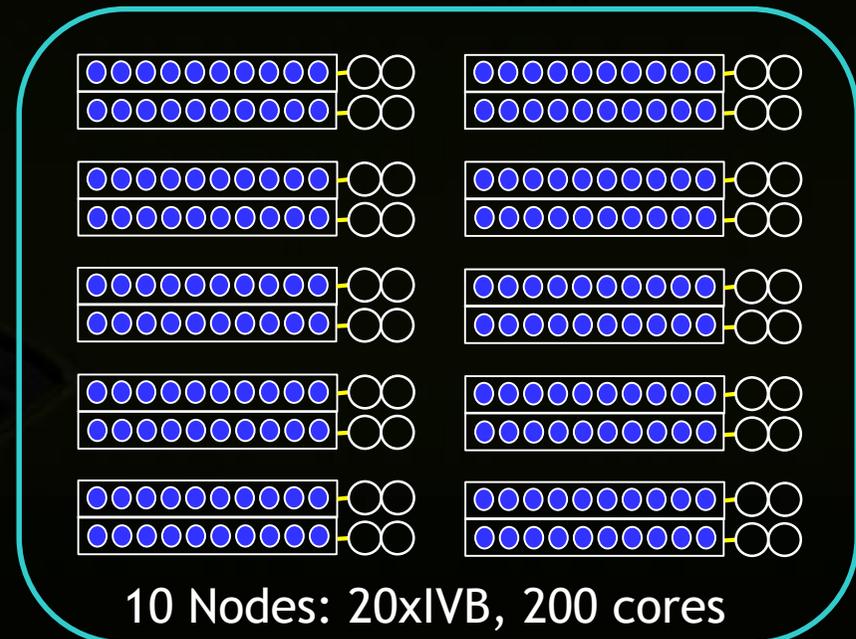
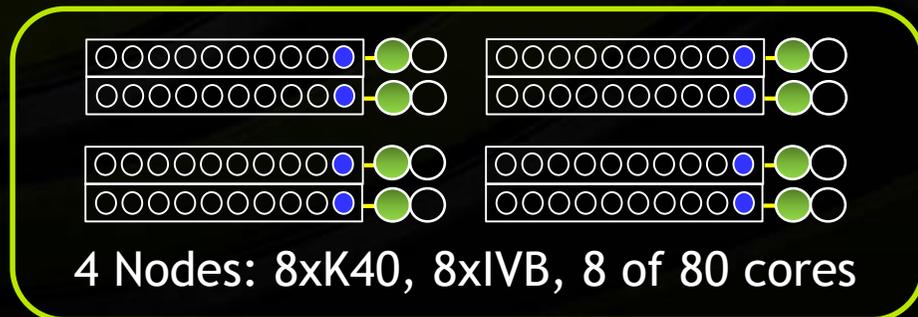
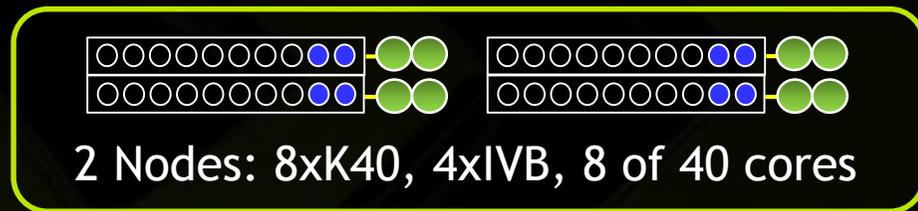
**ORCA025 settings:**

- Output every 5 days
- Total run: 10 days
- Time steps: 600
- NEMO 3.5

# NEMO HPC Configurations at Equal Performance

2 nodes + 8 GPUs = 4 nodes + 8 GPUs = 10 nodes

- Flexibility: GPUs free-up existing HPC nodes/cores for other applications
- Efficiency: GPU-based nodes more cost effective for new HPC purchase



# NICAM

## Recent Performance of NICAM on the K-Computer and Activities Towards Post-Petascale Computing

- Hisashi Yashiro(RIKEN), ECMWF Scalability Workshop, **Apr 2014**

Source: <http://www.ecmwf.int/newsevents/meetings/workshops/2014/Scalability/Presentations/pdfs/Yashiro.pdf>

## GPU optimization of global cloud resolving model NICAM core dynamics using OpenACC

- Hisashi Yashiro(RIKEN), GTC Japan, **Jul 2014**

Source: <http://www.gputechconf.jp/page/sessions.html>

# NICAM Performance with OpenACC and GPUs



## NICAM Model

<http://nicam.jp>

- Nonhydrostatic ICosahedral Atmospheric Model (2000 - Tomita and Satoh)
- Primary developers are JAMSTEC, University of Tokyo, and RIKEN AICS
- Collaborations: Athena project, COLA, ECMWF, NICS/UTK, ICOMEX
- Global resolution has high as 1.75 km achieved on K computer in Japan



## NICAM-DC Project

<http://scale.aics.riken.jp/nicamdc/>

- Dynamical core package of full NICAM full model - available as open source
- High order (3<sup>rd</sup>) advection scheme based on conservative semi-Lagrangian



## TSUBAME 2.5 System

<http://www.gsic.titech.ac.jp/en/tsubame>

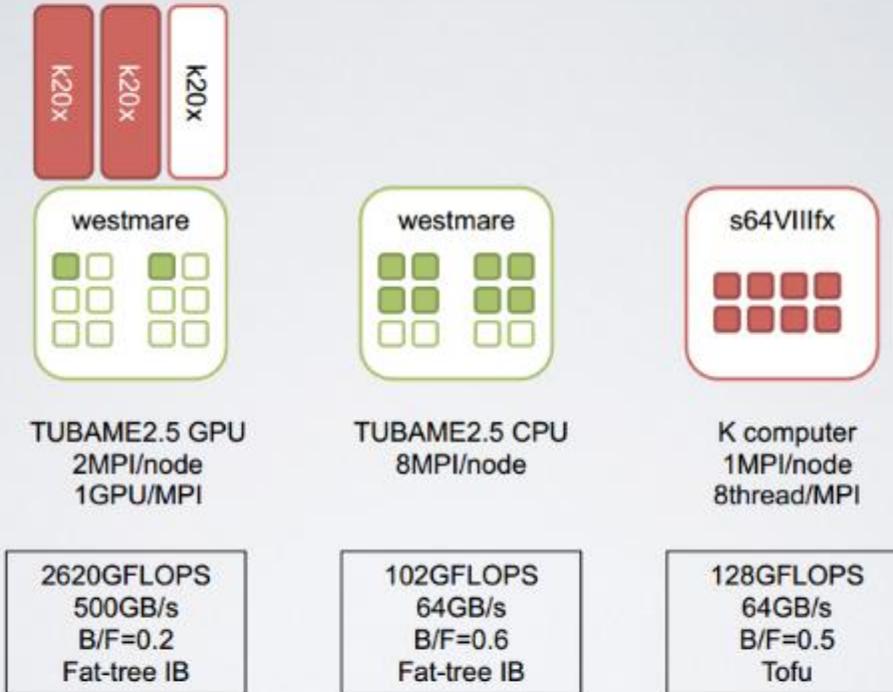
- TSUBAME 2.5 consists of 1408 compute nodes with 52 GB of system memory
- Each node 2 x Intel Xeon Westmere-EP 2.9 GHz CPUs and 3 x NVIDIA K20X GPUs
- NICAM tests on 5 nodes using 8 of 12 cores per node, and 2 of 3 GPUs per node



# NICAM Performance with OpenACC and GPUs



## Node-to-node comparison



**From the Workshop:  
ECMWF Scalability Project  
Apr 2014, Reading, UK**

***Recent Performance of  
NICAM on the K-Computer  
and Activities Towards  
Post-Petascale Computing***  
-by Dr. Hisashi Yashiro, RIKEN AICS

**TSUBAME 2.5  
Use of 2 cores + 2 GPUs  
vs. 8 of 12 cores per node**

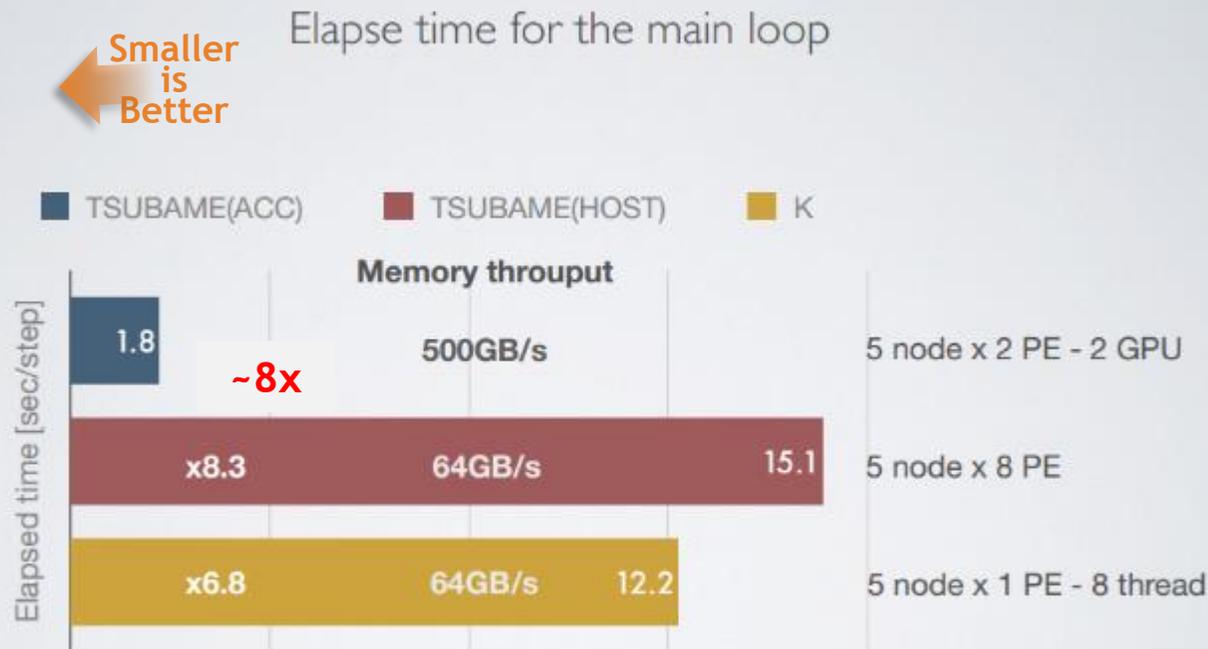


Source: <http://www.ecmwf.int/newsevents/meetings/workshops/2014/Scalability/Presentations/pdfs/Yashiro.pdf>

# NICAM Performance with OpenACC and GPUs



## Node-to-node comparison



From the Workshop:  
ECMWF Scalability Project  
Apr 2014, Reading, UK

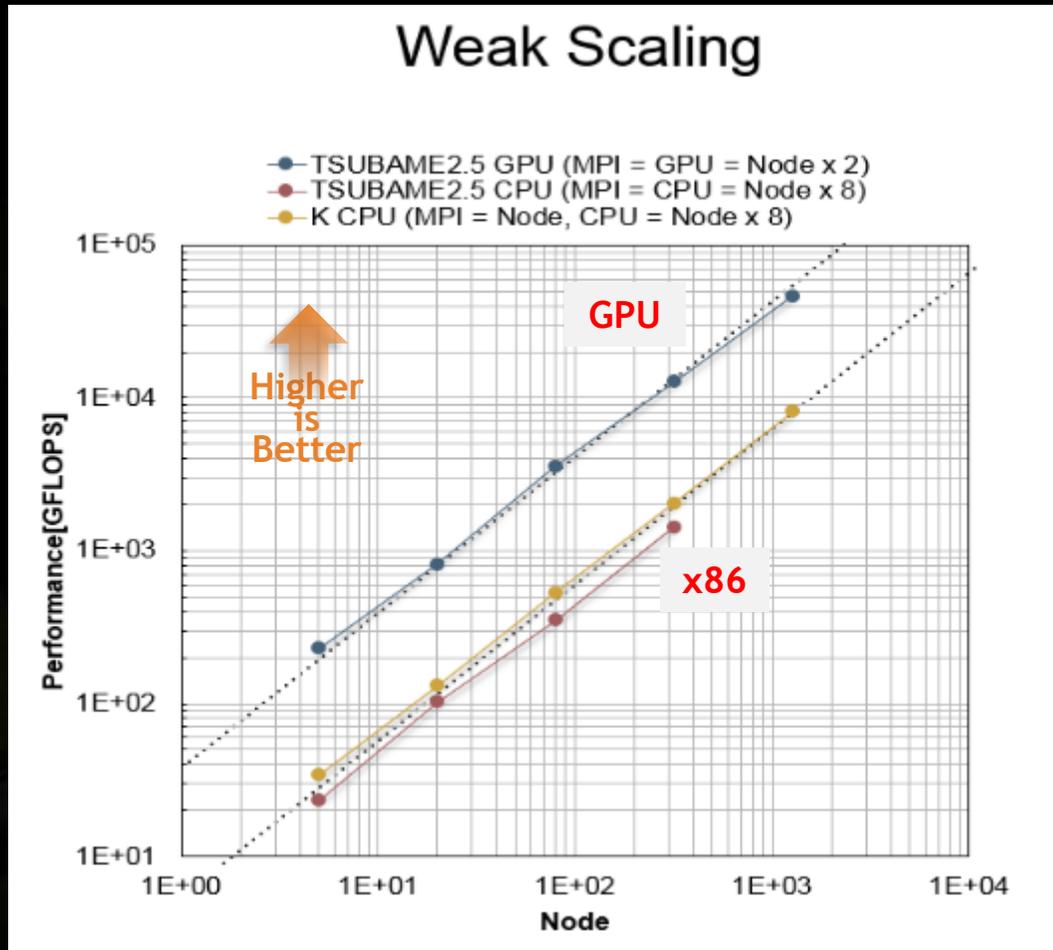
*Recent Performance of  
NICAM on the K-Computer  
and Activities Towards  
Post-Petascale Computing*  
-by Dr. Hisashi Yashiro, RIKEN AICS

Observed >8x speedup for  
dynamics using OpenACC  
on 5 nodes with 10 x K20X  
vs. 10 x Intel CPU (40 cores)



Source: <http://www.ecmwf.int/newsevents/meetings/workshops/2014/Scalability/Presentations/pdfs/Yashiro.pdf>

# NICAM Performance with OpenACC and GPUs



From the Workshop:  
ECMWF Scalability Project  
Apr 2014, Reading, UK

*Recent Performance of  
NICAM on the K-Computer  
and Activities Towards  
Post-Petascale Computing*  
-by Dr. Hisashi Yashiro, RIKEN AICS

**Observed GPU scaling to  
>1000 nodes (>2000 GPUs)**

Source: <http://www.ecmwf.int/newsevents/meetings/workshops/2014/Scalability/Presentations/pdfs/Yashiro.pdf>

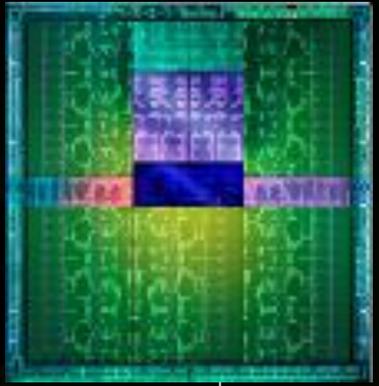
# Agenda: NVIDIA HPC Directions for ESM

- NVIDIA HPC and GPU Update
- ES Model Progress on GPUs
- **GPU Technology Roadmap**

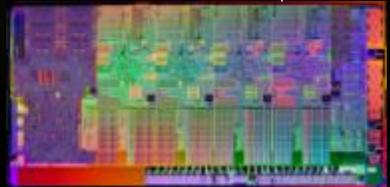
# New CPU Platforms Available During 2014



## Tesla K40 (Kepler)



PCIe - 16 GB/s



X86



ARM64

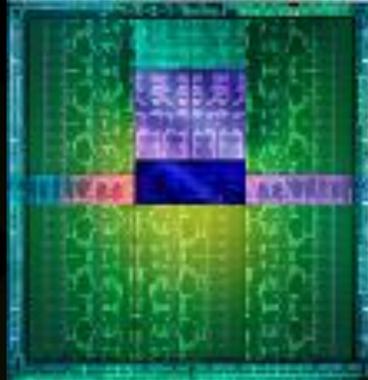


Power8

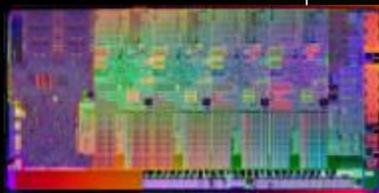
# Choice of CPU Platforms Available Starting 2016



## Pascal

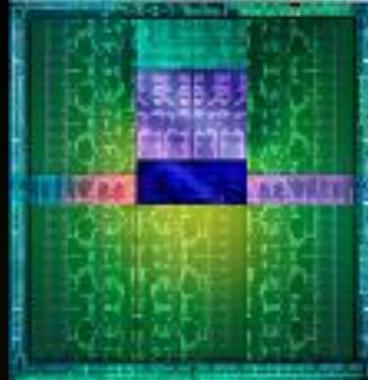


PCIe - 16 GB/s

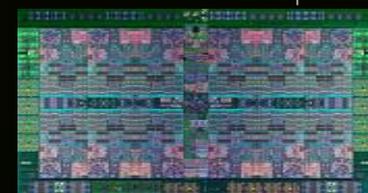


X86 | ARM64 | Power

## Pascal



NVLink - 80 GB/s



ARM64 | Power

# Features of Pascal GPU Architecture – 2016



## NVLink

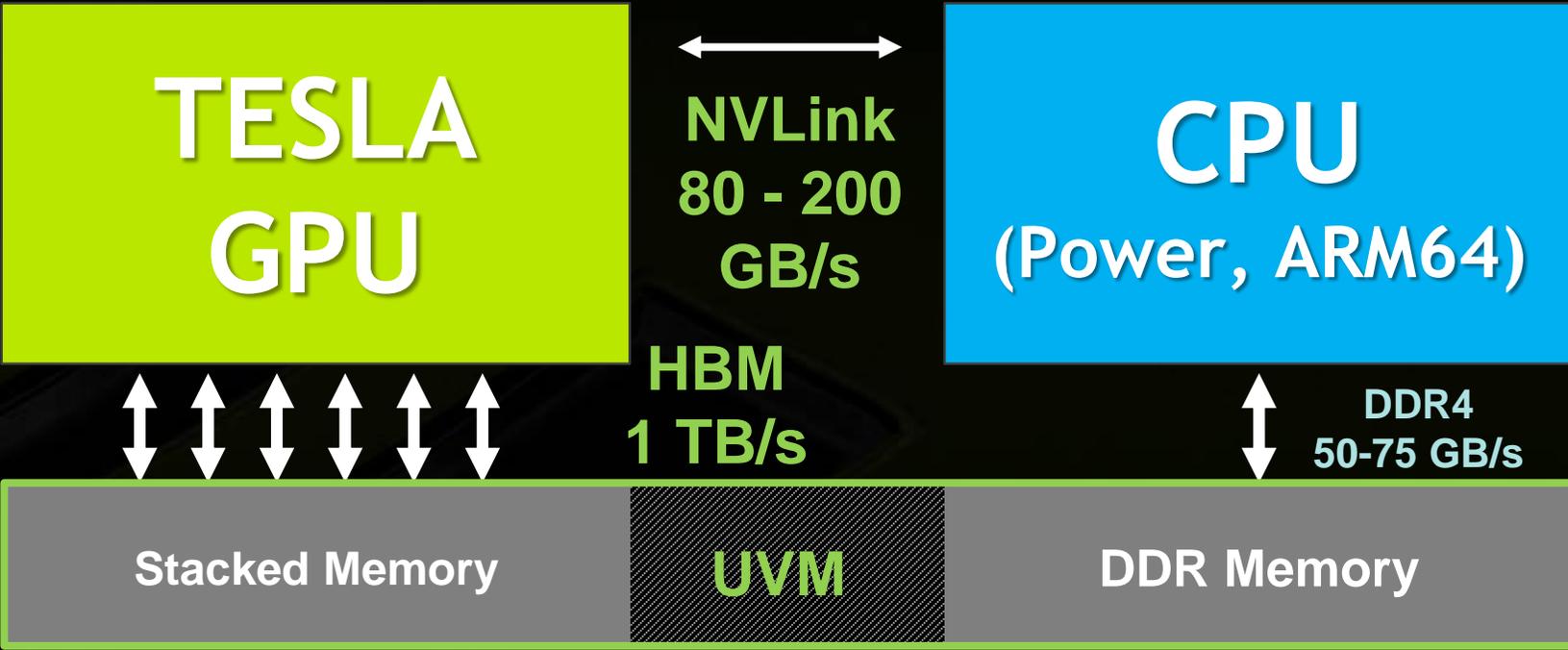
Interconnect at 80 GB/s  
(Speed of CPU Memory)

## Stacked Memory

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

## Unified Memory

Lower Development Effort  
(Available Today in CUDA6)



# Programming Strategies for GPU Acceleration



## Applications

**GPU Libraries**

Provides Fast  
“Drop-In”  
Acceleration

**OpenACC Directives**

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

**Programming Languages**

Maximum GPU  
Architecture  
Flexibility

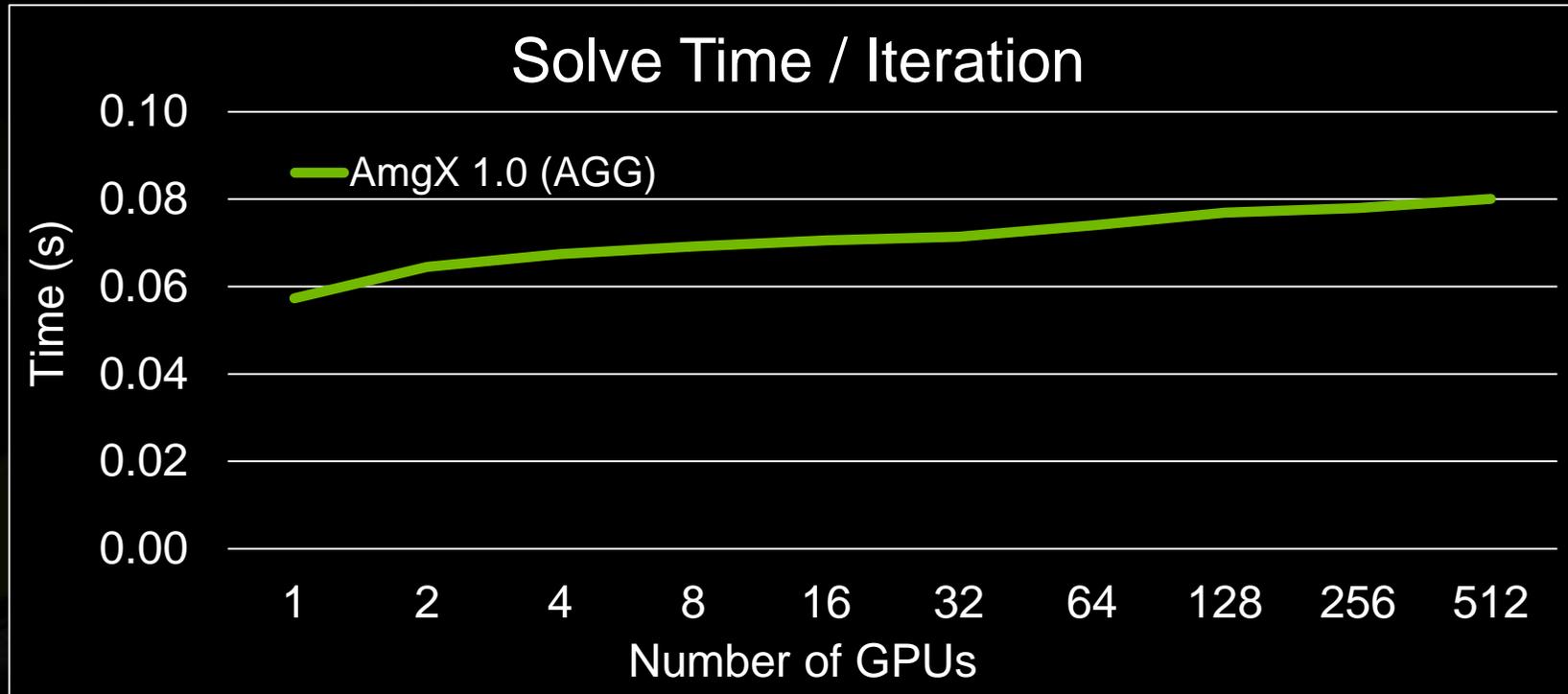


# NVIDIA AmgX for Iterative Implicit Methods

- Scalable linear solver library for  $Ax = b$  iterative methods
- No CUDA experience required, C API: links with Fortran, C, C++
- Reads common matrix formats (CSR, COO, MM)
- Interoperates easily with MPI, OpenMP, and hybrid parallel
- Single and double precision; Supported on Linux, Win64
- Multigrid; Krylov: GMRES, PCG, BiCGStab; Preconditioned variants
- Classic Iterative: Block-Jacobi, Gauss-Seidel, ILU's; Multi-coloring
- Flexibility: All methods as solvers, preconditioners, or smoothers
- Download AmgX library: <http://developer.nvidia.com/amgx>

# NVIDIA AmgX Weak Scaling on Titan 512 GPUs

Use of 512 nodes on ORNL TITAN System



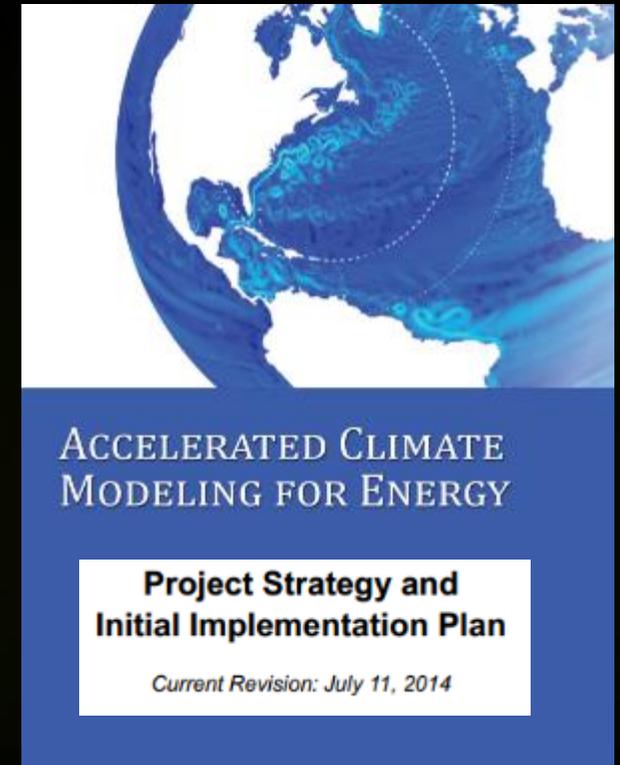
- Poisson matrix with ~8.2B rows solved in under 13 sec (200e3 Poisson matrix per GPU)
- ORNL TITAN: NVIDIA K20X one per node; CPU 16 core AMD Opteron 6274 @2.2GHz

# ACME: US DOE Accelerator-Based Climate Model



- **ACME: Accelerated Climate Model for Energy**
  - 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)
  - Towards NH global atm 12 km, ocn 15 km, 80 years
- **Co-design project with US DOE LCF systems**

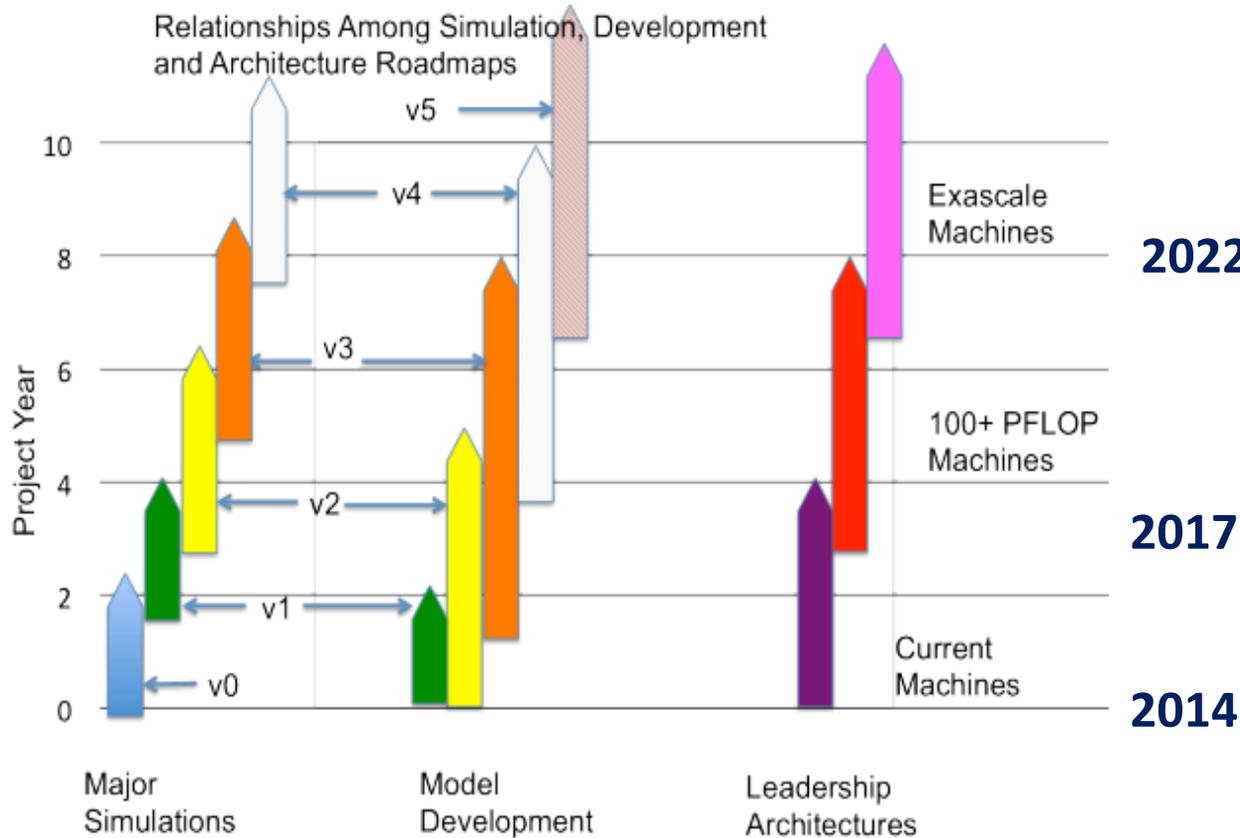
First Report – 11 Jul 2014



# ACME: US DOE Accelerator-Based Climate Model



## ACME Project Roadmap (page 2 in report)



- TBD

- **CORAL: ORNL – ANL – LLNL**  
[Systems to be announced SC14]

- **Trinity, NERSC8 (Cori)**

- **TITAN - ORNL [AMD + GPU]**

- **Mira – ANL [Blue GeneQ]**

# Summary Highlights: NVIDIA HPC Directions for ESM

- **NVIDIA observes strong ESM community interest in GPU acceleration**
  - New technologies: Pascal, NVLink, more CPU platform choices
  - NVIDIA business and engineering collaborations in 16 model projects
  - Investments in OpenACC: PGI release of 14.9; Continued Cray collaborations
- **GPU progress for several models – we examined a few of these**
  - MeteoSwiss developments towards COSMO operational NWP on GPUs
  - OpenACC for NICAM: 1 of 6 applications driving exascale plans at RIKEN, JP
  - OpenACC for NEMO: Leading ocean component model in ENES models
  - Ongoing GPU developments for 24 of 30 ES models where NVIDIA focus
- **Watch for announcements coming at Supercomputing'14, 17 Nov 2014**
  - New GPU products and technologies with further details on roadmap

# Thank you and Questions?

Stan Posey; [sposey@nvidia.com](mailto:sposey@nvidia.com); NVIDIA, Santa Clara, CA, USA