

NVIDIA DEVELOPMENTS FOR EARTH SYSTEM MODELING

Stan Posey, HPC Program Manager, ESM Domain, NVIDIA (HQ), Santa Clara, CA, USA



TOPICS OF DISCUSSION

- **NVIDIA HPC AND ESM UPDATE**
- **GPU TECHNOLOGY FOR ESM**

NVIDIA Company Introduction

HQ in Santa Clara, CA, USA

FY16 Revenue ~\$5B USD

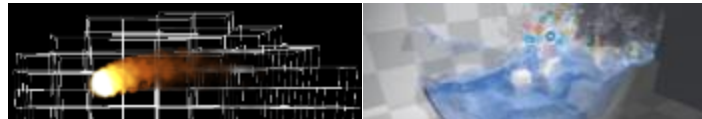
Employs ~9,500 in 20 Countries



NVIDIA Core Markets



GPU Computing

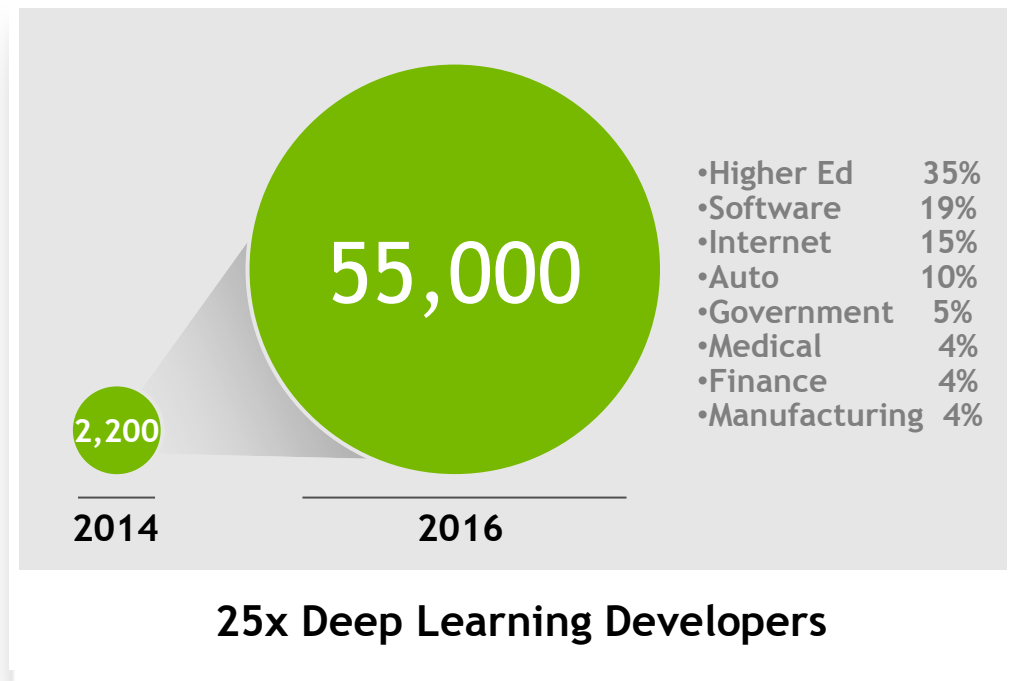
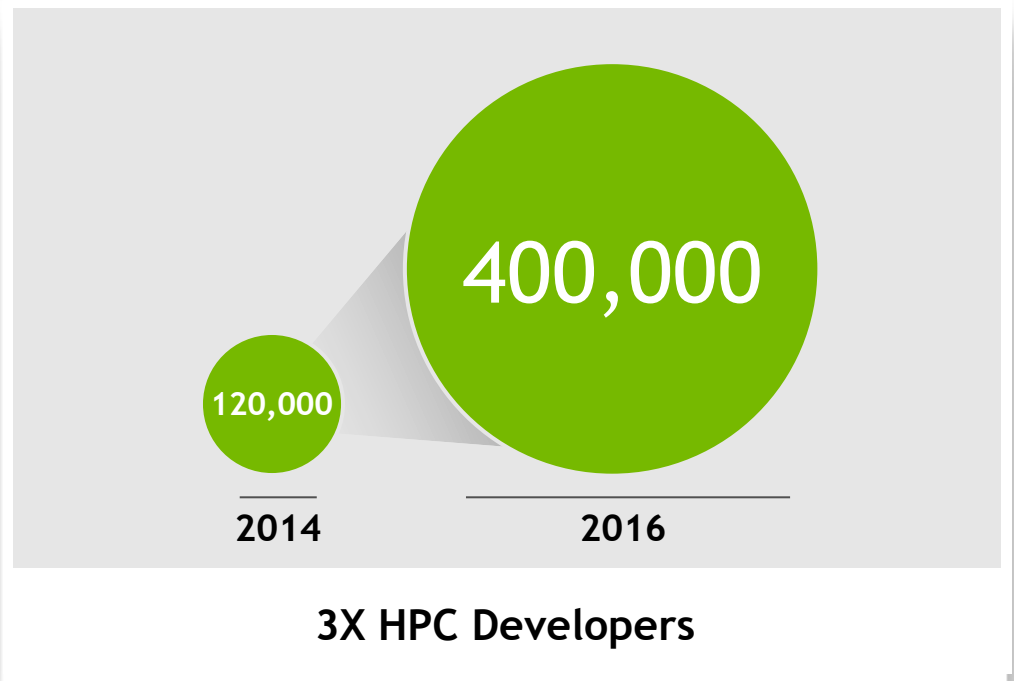


Computer Graphics



Artificial Intelligence

NVIDIA Growth from Advancement of HPC and AI

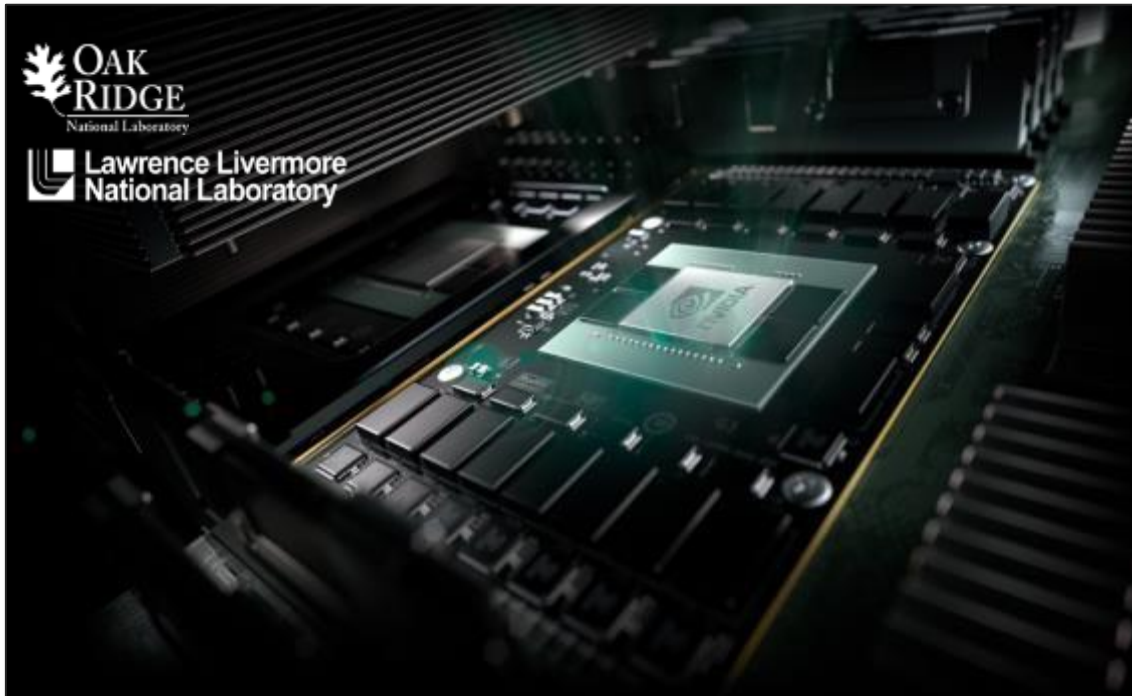


GPUs Power World's Leading Data Centers for HPC and AI:



HPC Advancements: US DOE Supercomputers

Pre-Exascale Systems Powered by NVIDIA Tesla



Summit & Sierra Supercomputers

150-300 PFLOPS Peak

Featuring NVIDIA Volta GPU

NVLink High Speed Interconnect

40 TFLOPS per Node, >3,400 Nodes

2018

RECENT NWP DEPLOYMENTS WITH GPU SYSTEMS

Cray CS-Storm, 192 x K80, 8 GPUs per node



MeteoSwiss Deploys World's 1st Operational NWP on GPUs

2-3x higher resolution for daily forecasts

14x more simulation with ensemble approach for medium-range forecasts

NWP Model: COSMO



Cray CS-Storm, 760 x P100, 8 GPUs per node



NOAA To Improve NWP and Climate Research with GPUs

Develop global model with 3km resolution, five-fold increase from today's resolution

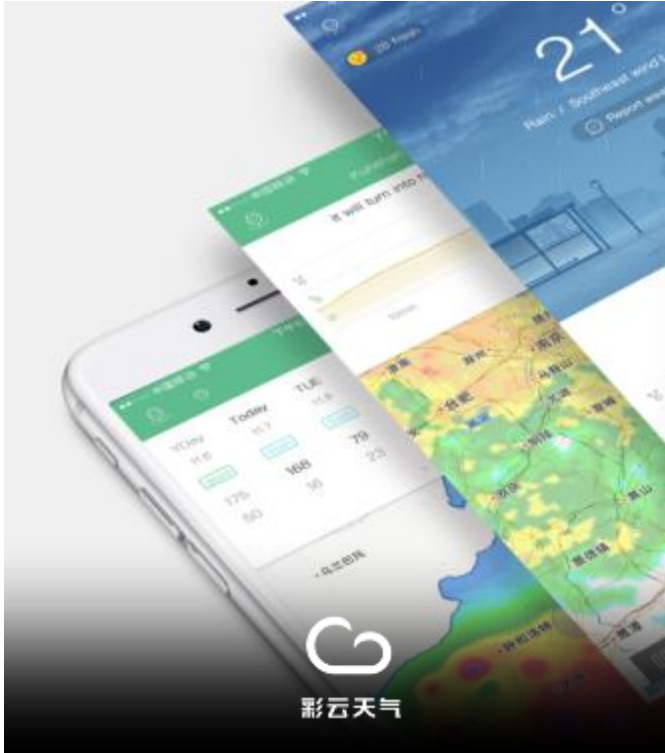
NWP Model: FV3/GFS (also climate research)



Deep Learning Growth in NWP and Observations



Monitoring Effects of Carbon and Greenhouse Gas Emissions



Colorful Clouds (CN) AI Weather Forecasting



Yandex
Meteum

DNN-Based Technology behind Yandex.Nowcasting

- › Innovative topology for CNN
- › Nets combine convolution/deconvolution, ResNet, and spatial transform layers

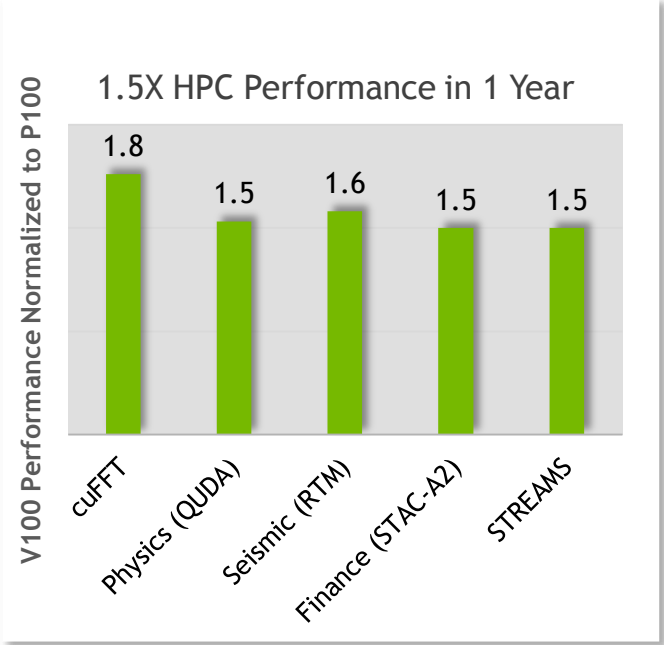
Yandex Meteum (RU) AI Hyperlocal Nowasting

NVIDIA Volta - Latest GPU Announced at GTC 2017

TESLA V100 SPECIFICATIONS



Compute	7.5 TF DP · 15 TF SP · 120 TF DL
Memory	HBM2: 900 GB/s · 16 GB
Interconnect	NVLink (up to 300 GB/s) + PCIe Gen3 (up to 32 GB/s)
Availability	DGX-1: Q3 2017; OEM : Q4 2017



System Config Info: 2X Xeon E5-2690 v4, 2.6GHz, w/ 1X Tesla P100 or V100. V100 measured on pre-production hardware.

Update on DOE Pre-Exascale CORAL Systems

- LLNL Sierra 150PF in 2018
- ORNL Summit 200PF in 2018
 - CAAR support from IBM and NVIDIA

TITAN VS SUMMIT

Compute System Comparison



FEATURE	TITAN	SUMMIT
Application Performance	Baseline	5-10x Titan
Number of Nodes	18,688	~4,600
Node performance	1.4 TF	> 40 TF
Memory per Node	32 GB DDR3 + 6 GB GDDR5	512 GB DDR4 + HBM
NV memory per Node	0	1600 GB
Total System Memory	710 TB	>10 PB DDR4 + HBM + Non-volatile
System Interconnect (node injection bandwidth)	Gemini (6.4 GB/s)	Dual Rail EDR-IB (23 GB/s)
Interconnect Topology	3d Torus	Non-blocking Fat Tree
Processors	1 AMD Opteron™ 1 NVIDIA Kepler™	2 IBM POWER9™ 6 NVIDIA Volta™
File System	32 PB, 1 TB/s, Lustre©	250 PB, 2.5 TB/s, GPFS™
Peak power consumption	9 MW	15 MW

~1/4x

~29x

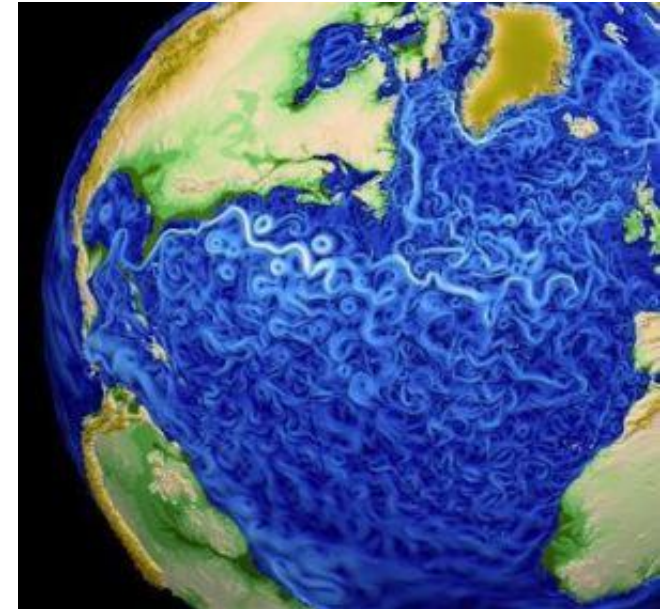
27,600 GPUs

~1.7x

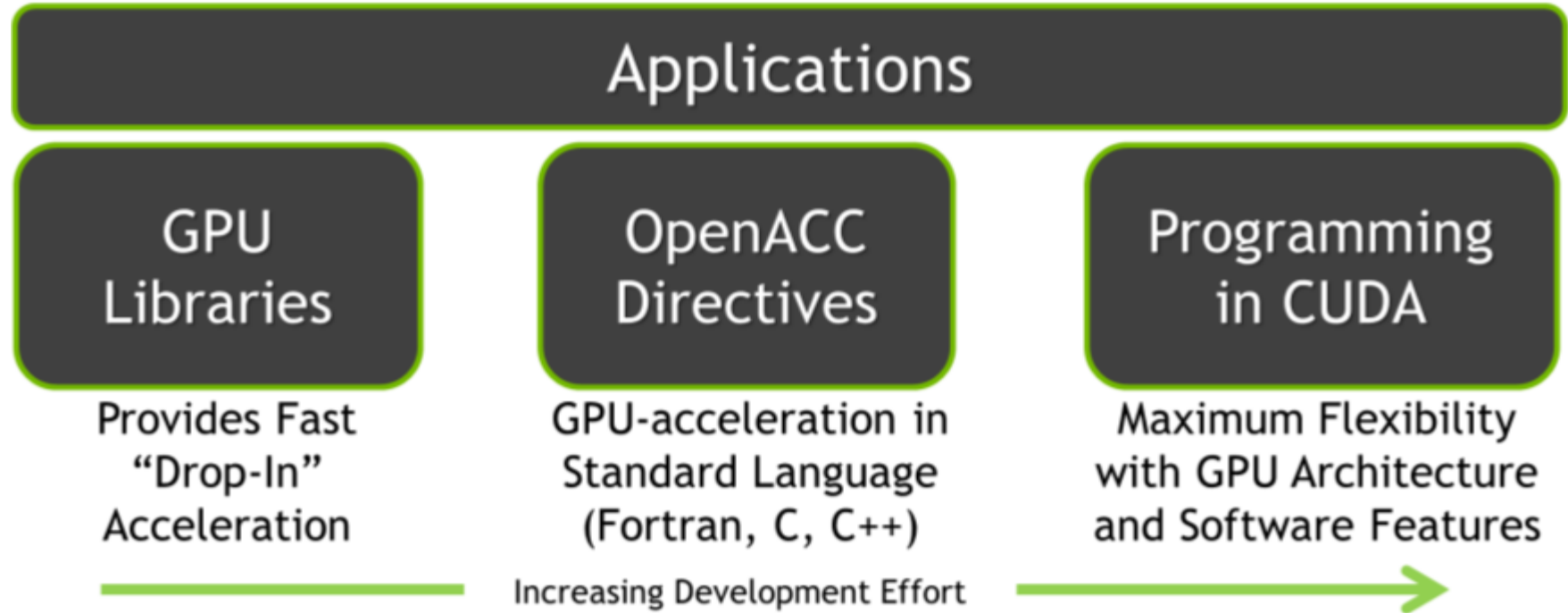


ACME Fully GPU-Accelerated Coupled Climate Model

- **ACME: Accelerated Climate Modeling 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
 - Towards NH global Atm 12 km, Ocn 15 km, 80 year
- **ACME component models and GPU progress**
 - Atm – ACME-Atmosphere (NCAR CAM-SE fork)
 - Dycore now in trunk, CAM physics started with OpenACC
 - Ocn – MPAS-O (LANL)
 - LANL team at ORNL OpenACC Hackathon during 2015
 - Others – published OpenACC progress
 - Sea-Ice – ACME-CICE (LANL)
 - Land – CLM (ORNL, NCAR)
 - Cloud Superparameterization – SAM (SBU, CSU)
 - Land-Ice – PISCEES (Multi-lab – LLNL, Sandia)



PROGRAMMING STRATEGIES FOR GPU ACCELERATION



NOTE: Many application developments include a combination of these strategies

Examples

- IFS (FFT, DGEMM)
- COSMO (Tridiag Solve)
- FV3
- MPAS
- IFS
- ICON
- COSMO (Physics)
- WRF -NCAR
- ACME
- CAM-SE
- NICAM
- ICON
- NEMO
- UM/Gungho
- COSMO (Dycore)
- NUMA
- ICON
- WRF -TQI
- NICAM (Dycore)

TOPICS OF DISCUSSION

- NVIDIA HPC AND ESM UPDATE
- **GPU TECHNOLOGY FOR NWP**
- DISCUSSION AND Q&A

Select NVIDIA ESM Highlights During 2016

- **WW ESM growth in GPU funded-development:** NOAA, NCAR, ECMWF, DOE, DoD
- **New ESM-driven GPU systems (K80/P100):** NOAA, ECMWF, CSCS, NIES, Others
- **First ever GPU-based operational NWP:** MeteoSwiss with COSMO (Mar 2016)
 - ~4x speedup with ~5x less energy vs. conventional CPU-only; New COSMO evaluations by Met's in DE, RU, IT
- **DOE climate model ACME-Atm v1 production on TITAN using PGI OpenACC**
- **New NCAR collaboration launched with GPU Hands-on Workshops**
 - <https://www2.cisl.ucar.edu/news/summertime-hackathon> (focus on GPU development of MPAS-A)
- **ECWMF selected NVIDIA as partner for ESCAPE Exascale weather project**
 - <https://software.ecmwf.int/wiki/display/OPTR/NVIDIA+Basic+GPU+Training+with+emphasis+on+Fortran+and+OpenACC>
- **NEMO Systems Team invited NVIDIA as member of HPC working group**
 - Following successful NVIDIA OpenACC scalability of NEMO for ORCA025 configuration (NEMO UGM 2014)
- **New ESM opportunities developing in new solution focus areas**
 - DL in climate and weather; BI for Ag and Actuary; Air quality monitoring (CN, KR); Commercial WRF start-up TQI
- **ESM model teams have consistent participation in GPU Hackathons**
 - DOE/ACME, NRL/COAMPS, MPI-M/ECHAM6, ODU/FVCOM, NRL/HYCOM, NOAA GFDL radiation models

GPU Funded-Development Growing for ESM

HPC Programs with Funding Specifically Targeted for GPU Development of Various ESMs



[SENA](#) - NOAA funding for accelerator development of **WRF**, NGGPS (**FV3**), **GFDL climate**, **NMMB**



[ESCAPE](#) - ECMWF-led EUC Horizon 2020 program for **IFS**; NVIDIA 1 of 11 funded partners



[ACME](#) - US DOE accelerated climate model: **CAM-SE**, **MPAS-O**, **CICE**, **CLM**, **SAM**, **PISCEES**, others



[AIMES](#) - Govt's from DE, FR, and JP for HPC (and GPU) developments of **ICON**, **DYNAMICO**, **NICAM**



[SIParCS](#) - NCAR academia funding for HPC (and GPU) developments of **MPAS**, **CESM**, **DART**, **Fields**



[AOLI](#) - US DoD accelerator development of operational models **HYCOM**, **NUMA**, **CICE**, **RRTMG**



[GridTools](#) - Swiss gov funding MCH/CSCS/ETH for accelerator-based DSL in **COSMO**, **ICON**, others

NOTE: Follow each program [LINK](#) for details; Programs listed from top-down in rough order of newest to oldest start date

GPUs Deployed for ESM and NWP Modeling (Apr 17)



Organization	Location	GPUs	System
DOE ORNL	Oak Ridge, TN, US	Volta – 200 PF	IBM Power9 – <i>Summit</i>
DOE LLNL	Livermore, CA, US	Volta – 150 PF	IBM Power9 – <i>Sierra</i>
CSCS	Lugano, CH	P100 – 4,500	Cray XC-40
NOAA	Fairmont, WV, US	P100 – 760	Cray CS-Storm
NIES	Tsukuba, JP	P100 – 266	HP/SGI ICE
DoD MHPCC	Maui, HI, US	P100 – 64	IBM Power8
MCH/CSCS	Lugano, CH	K80 – 192	Cray CS-Storm – <i>Piz Kesch</i>
ECMWF	Reading, UK	K80 – 68	Dell
DoD AFRL	Dayton, OH, US	K40 – 356	HP/SGI ICE X – <i>Thunder</i>
NASA GSFC	Greenbelt, MD, US	K40 – 36	HP/SGI, IBM x86
NASA ARC	Mtn View, CA, US	K40 – 64	HP/SGI – <i>Pleiades</i>
DOE ORNL	Oak Ridge, TN, US	K20X – 18,688	Cray – <i>TITAN</i>
CSCS	Lugano, CH	K20X – 5,272	Cray – <i>Piz Daint, Piz Dora</i>
TiTech	Tokyo, JP	K20X – 4,224	NEC/HP – <i>TSUBAME 2.0</i>
NCSA	Urb-Ch, IL, US	K20X – 3,072	Cray – <i>Blue Waters</i>
NCAR	Cheyenne, WY, US	K20X – 30	IBM x86 – <i>Yellowstone</i>


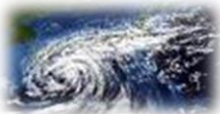
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GPU Developments for Atmospheric Models

	Organization	Location	Model	GPU Approach
Global 	ORNL, SNL	US	ACME-Atmosphere	OpenACC (migration from CUDA-F)
	ORNL, PNNL, UCI, SBU	US	SAM	OpenACC
	NCAR; THU	US	CAM-SE	OpenACC (migration from CUDA-F)
	NCAR, KISTI	US	MPAS-A	OpenACC
	NOAA GFDL, ESRL	US	FV3/GFS	OpenACC
	NASA GSFC	US	GEOS-5	OpenACC (migration from CUDA-F)
	US Naval Res Lab, NPS	US	NUMA/NEPTUNE	DSL – dycore only
	ECMWF	UK	IFS	Libs + OpenACC
	MetOffice , STFC	UK	UM/GungHo	OpenACC back-end to PSyKAI
	DWD, MPI-M, CSCS	DE, CH	ICON	DSL – dycore, OpenACC – physics
JAMSTEC, UT, RIKEN	JP	NICAM	OpenACC	
Regional 	NCAR; TQI/SSEC	US	WRF-ARW	(i) OpenACC, (ii) CUDA
	DWD, MCH, CSCS	DE, CH	COSMO	DSL – dycore, OpenACC – physics
	Bull, MF	FR	HARMONIE	OpenACC
	TiTech, JMA	JP	ASUCA	Hybrid-Fortran, OpenACC

GPU Developments for Ocean Models

Model	Organization(s)	GPU Development Status
MPAS-O	DOE LANL (US)	Ocean component model for ACME , OpenACC GPU development committed
POP	DOE LANL, NCAR (US)	No GPU plans at LANL; Paper published on GPU development by NUDT (CN)
HYCOM	NOPP, DoD NRL, NOAA NCEP, FSU, Others (US)	Funded OpenACC GPU development through AOLI ; Participation in 2015 Hackathon
MOM	NOAA GFDL (US)	Funded GPU development through SENA program, initial GPU profiling underway
NEMO	CNRS, Mercator, UKMO, NERC, CMCC, INGV (EU, UK)	NVIDIA-led OpenACC development results at GTC 2013 and 2014 NEMO Users meeting ; HPC working group (NVIDIA as a member) will evaluate GPU potential
GOcean	UKMO, STFC (UK)	Use of UKMO GungHo framework, GPU development led by NVIDIA Devtech
POM	Princeton, ODU (US)	GPU development led by Tsinghua University (CN), results in 2015 publication
MITgcm	MIT, NASA (US)	Early GPU investigations by MIT (C. Hill); nothing currently in development
LICOM	CAS-IAP/LASG (CN)	GPU development ongoing, led by NVIDIA Devtech
ROMS	UCLA, Rutgers (US)	Early CUDA GPU investigations by Cal Poly (C. Lupo), results at GTC 2013
ADCIRC	UNC, UND, Others (US)	GPU investigations ongoing for DGM formulations, potential use of HPCX
FVCOM	UMass (US)	Participation in 2015 Hackathon, evaluation of OpenACC and AmgX GPU solver library



PGI® COMPILERS
& TOOLS

PGI COMPILERS & TOOLS UPDATE

PGI Compilers for Heterogeneous Supercomputing, June 2017



AGENDA

PGI Overview

OpenACC Applications & Performance

OpenPOWER & Volta V100

OpenACC and CUDA Unified Memory

PGI — THE NVIDIA HPC SDK

Fortran, C & C++ Compilers

Optimizing, SIMD Vectorizing, OpenMP

Accelerated Computing Features

OpenACC Directives, CUDA Fortran

Multi-Platform Solution

X86-64 and OpenPOWER Multicore CPUs

NVIDIA Tesla GPUs

Supported on Linux, macOS, Windows

MPI/OpenMP/OpenACC Tools

Debugger

Performance Profiler

Interoperable with DDT, TotalView

PGI[®]

The Compilers & Tools
for Supercomputing



OPENACC IS FOR MULTICORE, MANYCORE & GPUS

```
98 !$ACC KERNELS
99 !$ACC LOOP INDEPENDENT
100     DO k=y_min-depth,y_max+depth
101 !$ACC LOOP INDEPENDENT
102     DO j=1,depth
103         density0(x_min-j,k)=left_density0(left_xmax+1-j,k)
104     ENDDO
105 ENDDO
106 !$ACC END KERNELS
```

CPU

GPU

```
% pgfortran -ta=multicore -fast -Minfo=acc -c \
update_tile_halo_kernel.f90
```

```
. . .
100, Loop is parallelizable
    Generating Multicore code
    100, !$acc loop gang
102, Loop is parallelizable
```

```
% pgfortran -ta=tesla,cc35,cc60 -fast -Minfo=acc -c \
update_tile_halo_kernel.f90
```

```
. . .
100, Loop is parallelizable
102, Loop is parallelizable
    Accelerator kernel generated
    Generating Tesla code
    100, !$acc loop gang, vector(4) ! blockidx%y threadidx%y
    102, !$acc loop gang, vector(32) ! blockidx%x threadidx%x
```

CLOVERLEAF V1.3



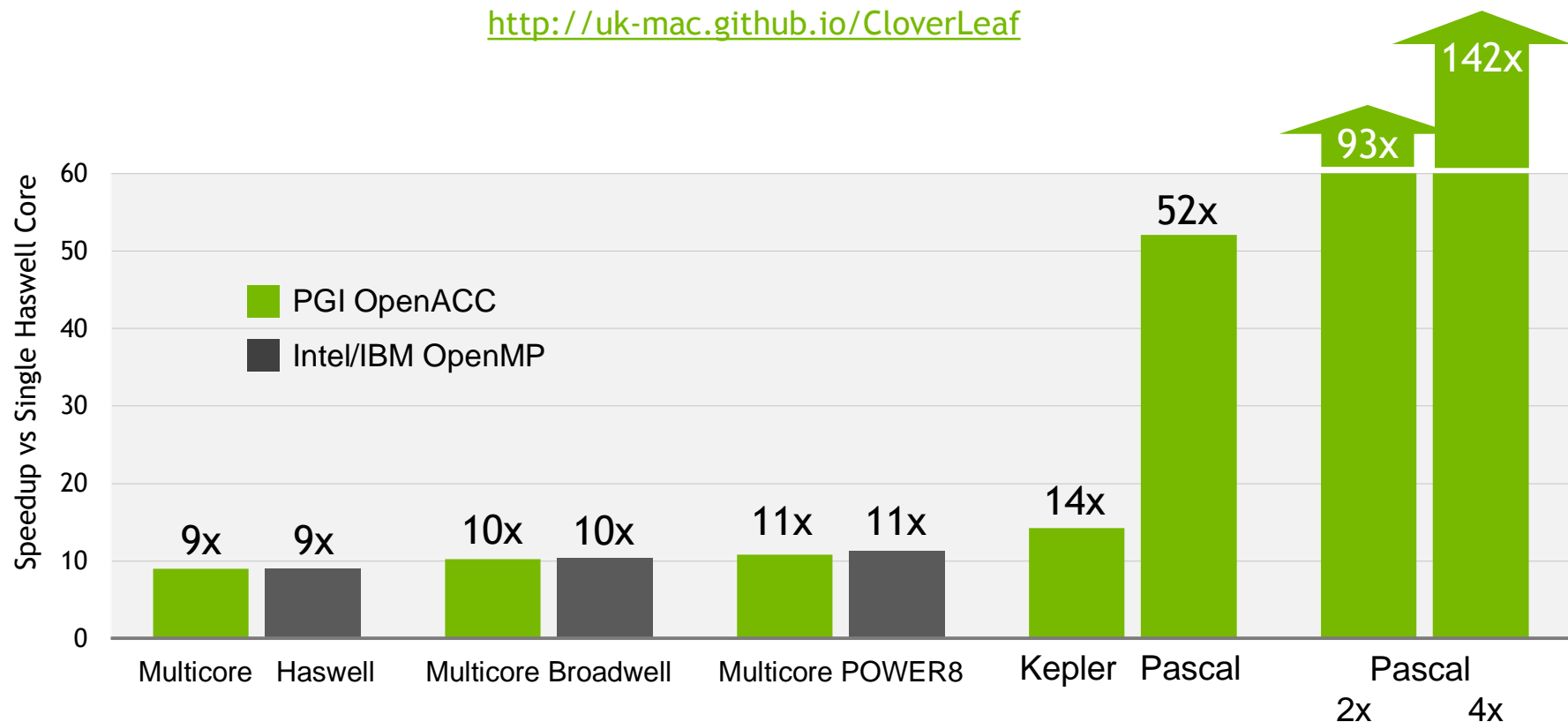
AWE Hydrodynamics mini-app
6500+ lines, !\$acc kernels
OpenACC or OpenMP
Source on GitHub

<http://uk-mac.github.io/CloverLeaf>

OPENACC PERFORMANCE PORTABILITY

AWE Hydrodynamics CloverLeaf mini-App, bm32 data set

<http://uk-mac.github.io/CloverLeaf>



Systems: Haswell: 2x16 core Haswell server, four K80s, CentOS 7.2 (perf-hsw10), Broadwell: 2x20 core Broadwell server, eight P100s (dgx1-prd-01), Minsky: POWER8+NVLINK, four P100s, RHEL 7.3 (gsn1).
Compilers: Intel 17.0.1, IBM XL 13.1.3, PGI 16.10.
Benchmark: CloverLeaf v1.3 downloaded from <http://uk-mac.github.io/CloverLeaf> the week of November 7 2016; CloverLeaf_Serial; CloverLeaf_ref (MPI+OpenMP); CloverLeaf_OpenACC (MPI+OpenACC)
Data compiled by PGI November 2016.

PGI COMPILERS & TOOLS FOR EVERYONE

PGI Community Edition Now Available

	FREE PGI [®] Community EDITION	PGI [®] Professional EDITION	PGI [®] Enterprise EDITION
PROGRAMMING MODELS OpenACC, CUDA Fortran, OpenMP, C/C++/Fortran Compilers and Tools	✓	✓	✓
PLATFORMS X86, OpenPOWER, NVIDIA GPU	✓	✓	✓
UPDATES	1-2 times a year	6-9 times a year	6-9 times a year
SUPPORT	User Forums	PGI Support	PGI Premier Services
LICENSE	Annual	Perpetual	Volume/Site

PGI 2017 NEW FEATURES

Fortran/C/C++ OpenACC 2.5 on Tesla GPUs and multicore CPUs

- CUDA 8.0/P100 GPU accelerator support
- OpenACC for multicore Haswell, Broadwell and OpenPOWER CPUs
- User-driven OpenACC performance optimizations

Full C++ 14 language support, interoperable with GCC/g++ 5.1 thru 6.2

OpenMP 4.5 Fortran for OpenPOWER multicore CPUs (no target offload, yet)

Multicore CPU Performance Optimizations

- OpenPOWER performance enhancements averaging 5-10%
- New tuned numerical intrinsics for Haswell/Broadwell
- Improved inlining

Updated OpenMPI, NetCDF, ESMF libraries; new OS distro's support; debugger enhancements

Full list of new features at www.pgicompilers.com/whats-new

... COMING SOON

OpenACC enhancements

- Deep copy of aggregate data structures
- CUDA Unified Memory enhancements
- GPU loop scheduling optimizations

New processors and platforms

- NVIDIA Volta V100 GPUs
- CUDA 9.0 support
- POWER9, Xeon Skylake, Xeon Phi KNL (Beta)

OpenMP 4.5 Fortran/C/C++ for Multicore CPUs (no target offload)

C++ atomics/abstraction performance, initial C++17, GNU 6.3 interop

Tools - OpenACC profiling, PGDBG/AVX-512, OpenPOWER DWARF gen

AGENDA

PGI Overview

OpenACC Applications & Performance

OpenPOWER & Volta V100

OpenACC and CUDA Unified Memory

OPENACC ADOPTION

NEW PLATFORMS



Sunway TaihuLight
#1 Top 500, Nov. 2016

GROWING COMMUNITY



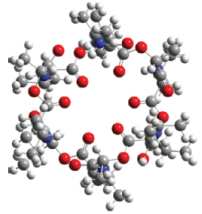
- 6,000+ enabled developers
- 4,500+ course registrants
- 350+ Hackathon attendees
- 150+ User Group members

PORTING SUCCESS

- Gaussian 16 ported to Tesla with OpenACC
- Five of 13 ORNL CAAR codes using OpenACC
- ANSYS Fluent R18 production release is GPU accelerated using OpenACC

GAUSSIAN 16

A Leading Computation Chemistry Code



Valinomycin
wB97xD/6-311+(2d,p) Freq
2.25X speedup

Hardware: HPE server with dual Intel Xeon E5-2698 v3 CPUs (2.30GHz ; 16 cores/chip), 256GB memory and 4 Tesla K80 dual GPU boards (boost clocks: MEM 2505 and SM 975). Gaussian source code compiled with PGI Accelerator Compilers (16.5) with OpenACC (2.5 standard).



Mike Frisch, Ph.D.
President and CEO
Gaussian, Inc.



Using OpenACC allowed us to continue development of our fundamental algorithms and software capabilities simultaneously with the GPU-related work. In the end, we could use the same code base for SMP, cluster/network and GPU parallelism. PGI's compilers were essential to the success of our efforts.

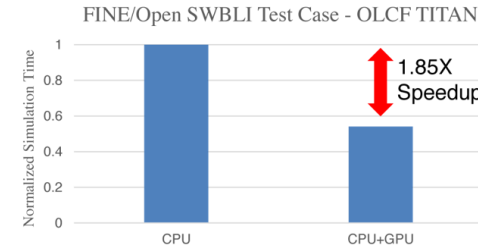


NUMECA FINE/OPEN

Unstructured CDF Solver



David Gutzwiller
Lead Software Developer
NUMECA



System: Four nodes on the OLCF Titan supercomputer (16 cores and 1 GPU per node).



ANSYS FLUENT

Discrete Ordinate (DO) Radiation Solver



Sunil Sathe
Lead Software Developer
ANSYS Fluent



We've effectively used OpenACC for heterogeneous computing in ANSYS Fluent with impressive performance. We're now applying this work to more of our models and new platforms.



MPAS ATMOSPHERE

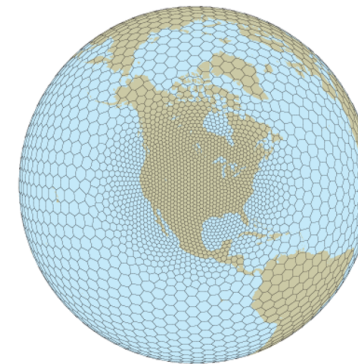
Climate and Weather Modeling



Richard Loft
Director, Technology Development
NCAR



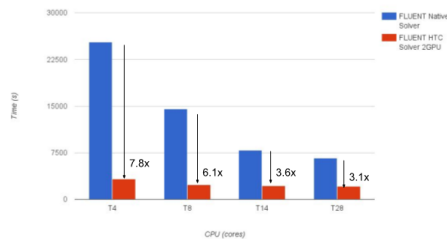
Our team has been evaluating OpenACC as a pathway to performance portability for the Model for Prediction (MPAS) atmospheric model. Using this approach on the MPAS dynamical core, we have achieved performance on a single P100 GPU equivalent to 2.7 dual socketed Intel Xeon nodes on our new Cheyenne supercomputer.



A variable resolution MPAS Voronoi mesh

Source: mpas.github.io
<https://mpas-dev.github.io/atmosphere/atmosphere.html>

GPU vs CPU Speed-up



CPU Hardware:
(Haswell EP) Intel(R) Xeon(R) CPU E5-2695 v3 @ 2.30GHz, 2 socket x 14 = 28 cores
GGPU Hardware:
Tesla K80 12+12 GB, Driver 346.46

COSMO

Regional Atmospheric Model



Image courtesy Meteoswiss.



Dr. Oliver Fuhrer
Senior Scientist
Meteoswiss

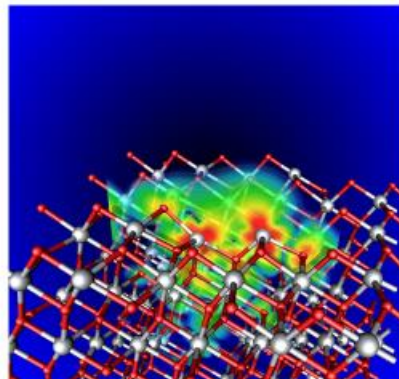


OpenACC made it practical to develop for GPU-based hardware while retaining a single source for almost all the COSMO physics code.



VASP

The Vienna Ab Initio Simulation Package



Dr. Martijn Marsman
Computational Materials Physics
University of Vienna



Early indications are that we can nearly match the performance of CUDA using OpenACC on GPUs. This will enable our domain scientists to work on a uniform GPU accelerated Fortran source code base.



PGI

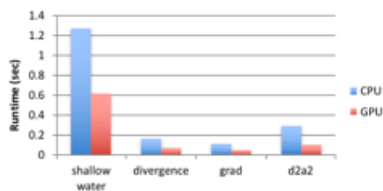
PGI

FV3 WEATHER MODEL

Global Weather Forecast Model

OpenACC Performance

- PGI compiler V16.10
- 2X faster performance on GPU
- Dual-socket Haswell CPU and NVIDIA Pascal (P100) GPU



Slide courtesy of Mark Govett,
NOAA / Earth System Research Laboratory



Mark Govett
Chief, HPC Section
NOAA

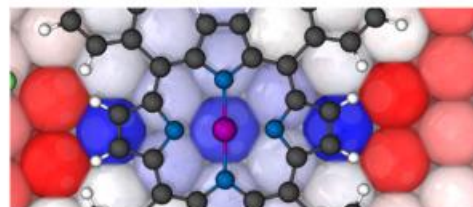


Lessons learned in the development of NIM and F2C-ACC have proven invaluable in our current efforts to create a single, performance portable version of the FV3 weather model using OpenACC.



QUANTUM ESPRESSO

Quantum Chemistry Suite



Filippo Spiga
Head of Research Software Engineering
University of Cambridge



CUDA Fortran gives us the full performance potential of the CUDA programming model and NVIDIA GPUs. !\$CUFF KERNELS directives give us productivity and source code maintainability. It's the best of both worlds.



www.quantum-espresso.org

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AGENDA

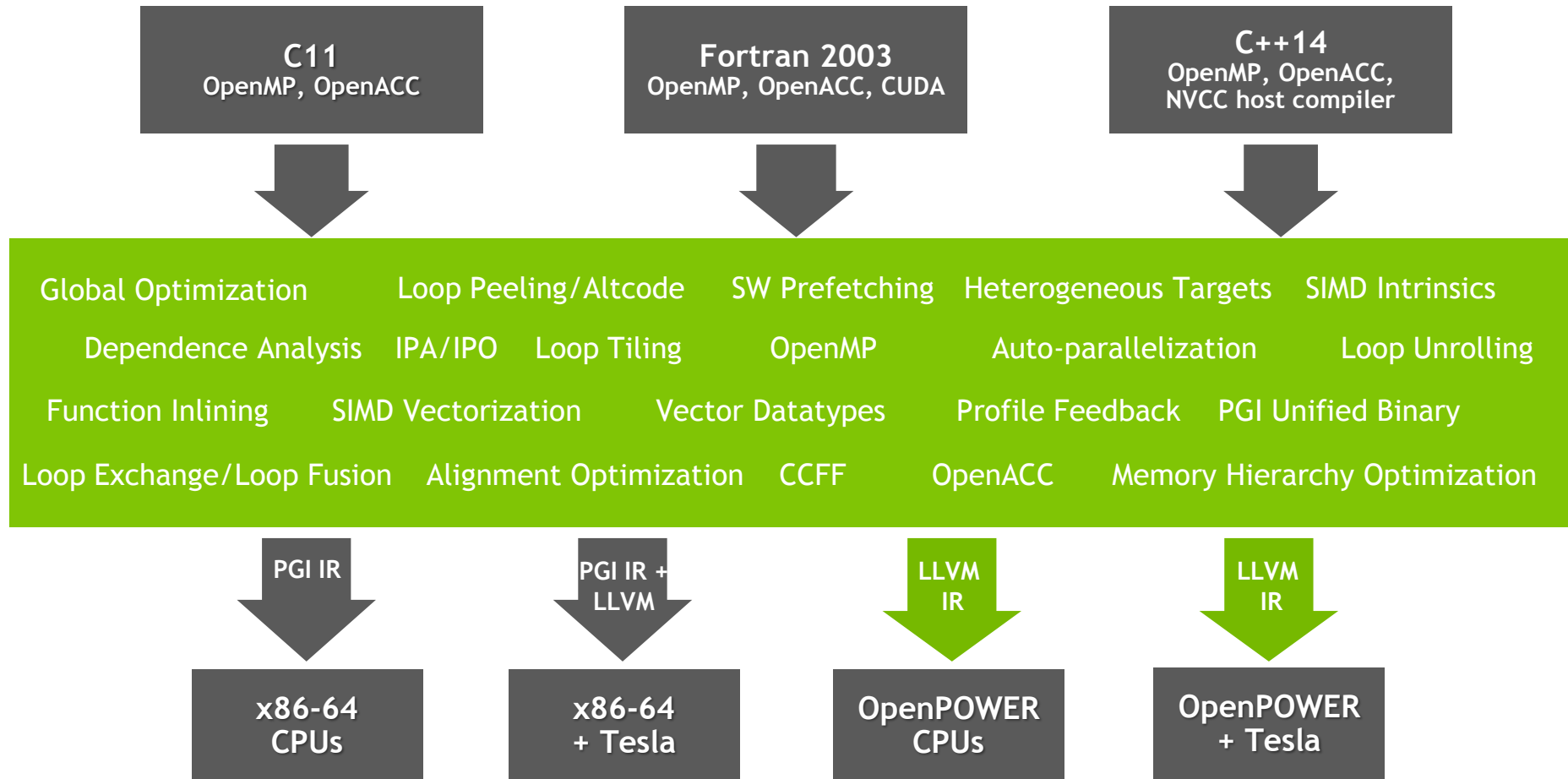
PGI Overview

OpenACC Applications & Performance

OpenPOWER & Volta V100

OpenACC and CUDA Unified Memory

The PGI Compiler Infrastructure



PGI FOR OpenPOWER+TESLA

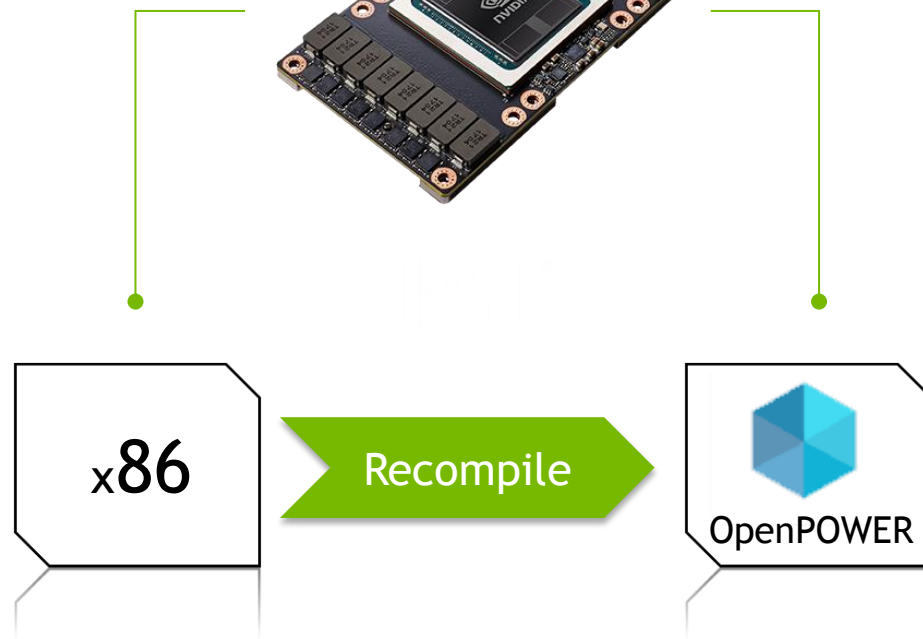
Fortran 2003, C11, C++14 compilers,
performance profiler

CUDA Fortran, OpenACC, OpenMP,
NVCC host compiler

Integrated IBM-optimized LLVM
OpenPOWER code generator

Available now at:

pgicompilers.com/openpower



PGI FOR OpenPOWER+TESLA

Fortran 2003, C11, C++14 compilers,
performance profiler

CUDA Fortran, OpenACC, OpenMP,
NVCC host compiler

Integrated IBM-optimized LLVM
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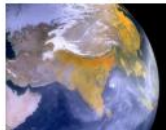
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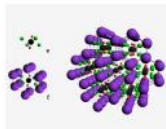
Center for Accelerated Application Readiness (CAAR)

In preparation for next-generation supercomputer Summit, the Oak Ridge Leadership Computing Facility (OLCF) selected 13 partnership projects into its Center for Accelerated Application Readiness (CAAR) program. A collaborative effort of application development teams and staff from the OLCF Scientific Computing group, CAAR is focused on redesigning, porting, and optimizing application codes for Summit's hybrid CPU-GPU architecture. Through CAAR, codes teams gain access to early software development systems, leadership computing resources, and technical support from the IBM/NVIDIA Center of Excellence at Oak Ridge National Laboratory. The program culminates with each team's scientific grand-challenge demonstration on Summit. The modeling and simulation applications selected for the CAAR program include:



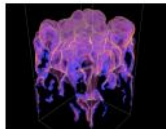
Code: ACME
Science Domain: Climate
Title: Climate Research: Advancing Earth System Models
PI: David Bader, Lawrence Livermore National Laboratory

[Learn More](#)



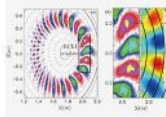
Code: DIRAC
Science Domain: Relativistic Quantum Chemistry
Title: CAAR Oak Ridge Proposal for getting the Relativistic Quantum Chemistry Program Package DIRAC ready for SUMMIT
PI: Lucas Visscher, Amsterdam Center for Multiscale Modeling /VU University Amsterdam

[Learn More](#)



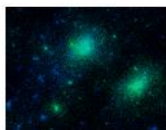
Code: FLASH
Science Domain: Astrophysics
Title: Using FLASH for Astrophysics Simulations at an Unprecedented Scale
PI: Bronson Messer, Oak Ridge National Laboratory

[Learn More](#)



Code: GTC
Science Domain: Plasma Physics
Title: Particle Turbulence Simulations for Sustainable Fusion Reactions in ITER
PI: Zhihong Lin, University of California-Irvine

[Learn More](#)



Code: HACC
Science Domain: Cosmology
Title: Cosmological Simulations for Large-scale Sky Surveys
PI: Salman Habib, Argonne National Laboratory

[Learn More](#)



EVENTS CALENDAR

← OCTOBER 2016 →

M	T	W	T	F	S	S
26	27	28	29	30	1	2
3	4	5	6	7	8	9
10	11	12	13	14	15	16
17	18	19	20	21	22	23
24	25	26	27	28	29	30
31	1	2	3	4	5	6

WED 26 2016 GPU Hackathons
 January 1 @ 8:00 am - December 31 @ 5:00 pm

CENTER FOR ACCELERATED APPLICATION READINESS (CAAR)

Oak Ridge Leadership Computing Facility

Collaboration of application development teams and OLCF staff focused on redesigning, porting, and optimizing 13 application codes for Summit's hybrid POWER9+Volta node architecture.

www.olcf.ornl.gov/caar

X86-64 TO OPENPOWER PORTING

C/C++ ABI DIFFERENCES

signed vs unsigned default char
long double

NUMERICAL DIFFERENCES

Intrinsics accuracy may differ
across targets
FMA vs. no FMA

PLATFORM DIFFERENCES

Large memory model
C varargs

X86-SPECIFIC FEATURES

Inline *asm* statements
SSE/AVX intrinsics

NVIDIA TESLA V100 GPU

GIANT LEAP FOR AI & HPC

5,120 CUDA cores | 640 Tensor cores

7.5 FP64 TFLOPS | 15 FP32 TFLOPS

NEW 120 Tensor TFLOPS

20MB SM RF | 16MB Cache

16GB HBM2 @ 900 GB/s

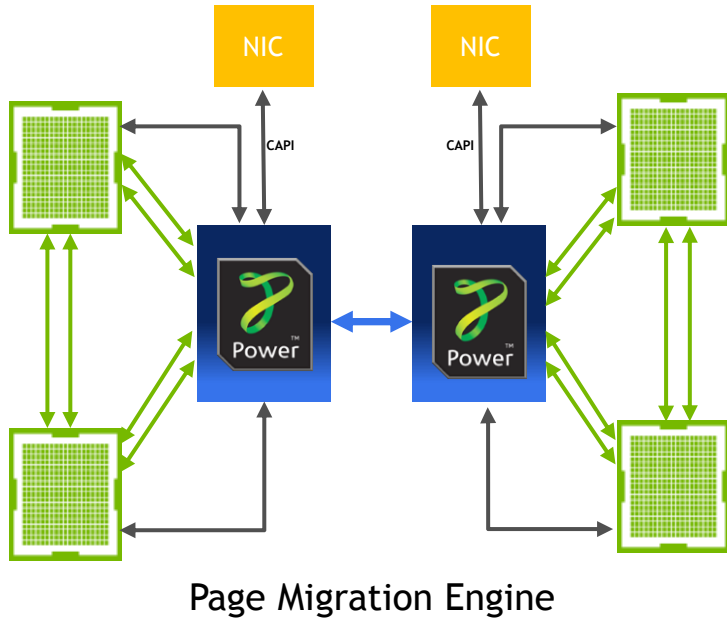
300 GB/s NVLink



IBM POWER NVLINK SYSTEMS

APPROVED DESIGNS FOR OPENPOWER ECOSYSTEM

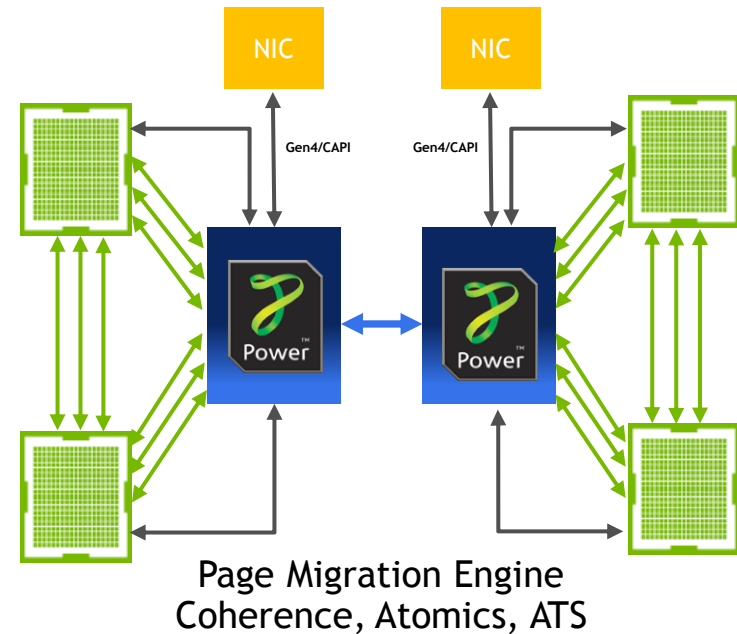
4 GPU POWER8 FOR PASCAL



P100 SXM2

40 GB/s full duplex each CPU:GPU and GPU:GPU link
IBM POWER8+ CPU

4 GPU POWER9 FOR VOLTA

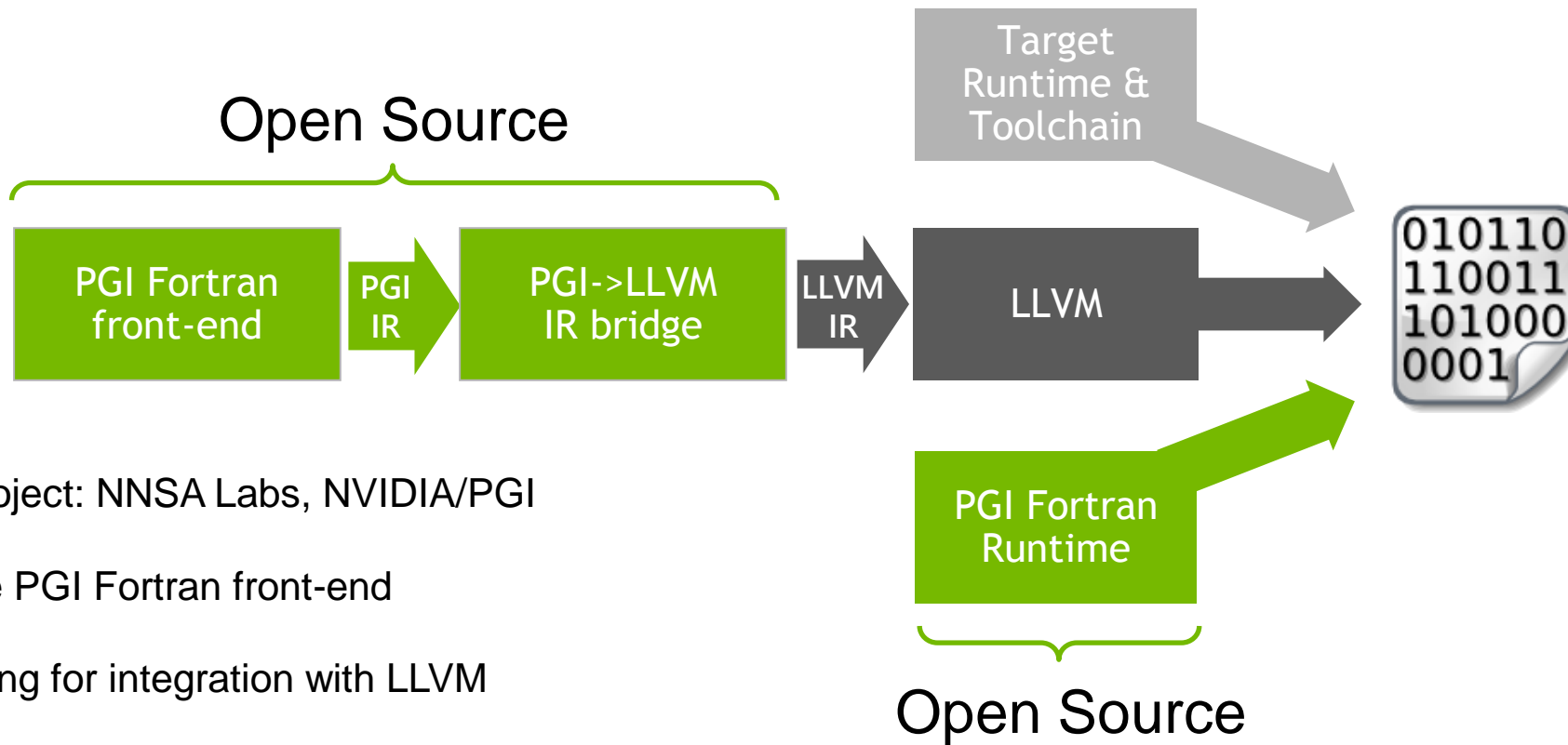


VOLTA SXM2

75 GB/s full duplex each CPU:GPU and GPU:GPU link
IBM POWER9 CPU

THE FLANG PROJECT

An open source Fortran front-end for LLVM



Multi-year project: NNSA Labs, NVIDIA/PGI

Based on the PGI Fortran front-end

Re-engineering for integration with LLVM

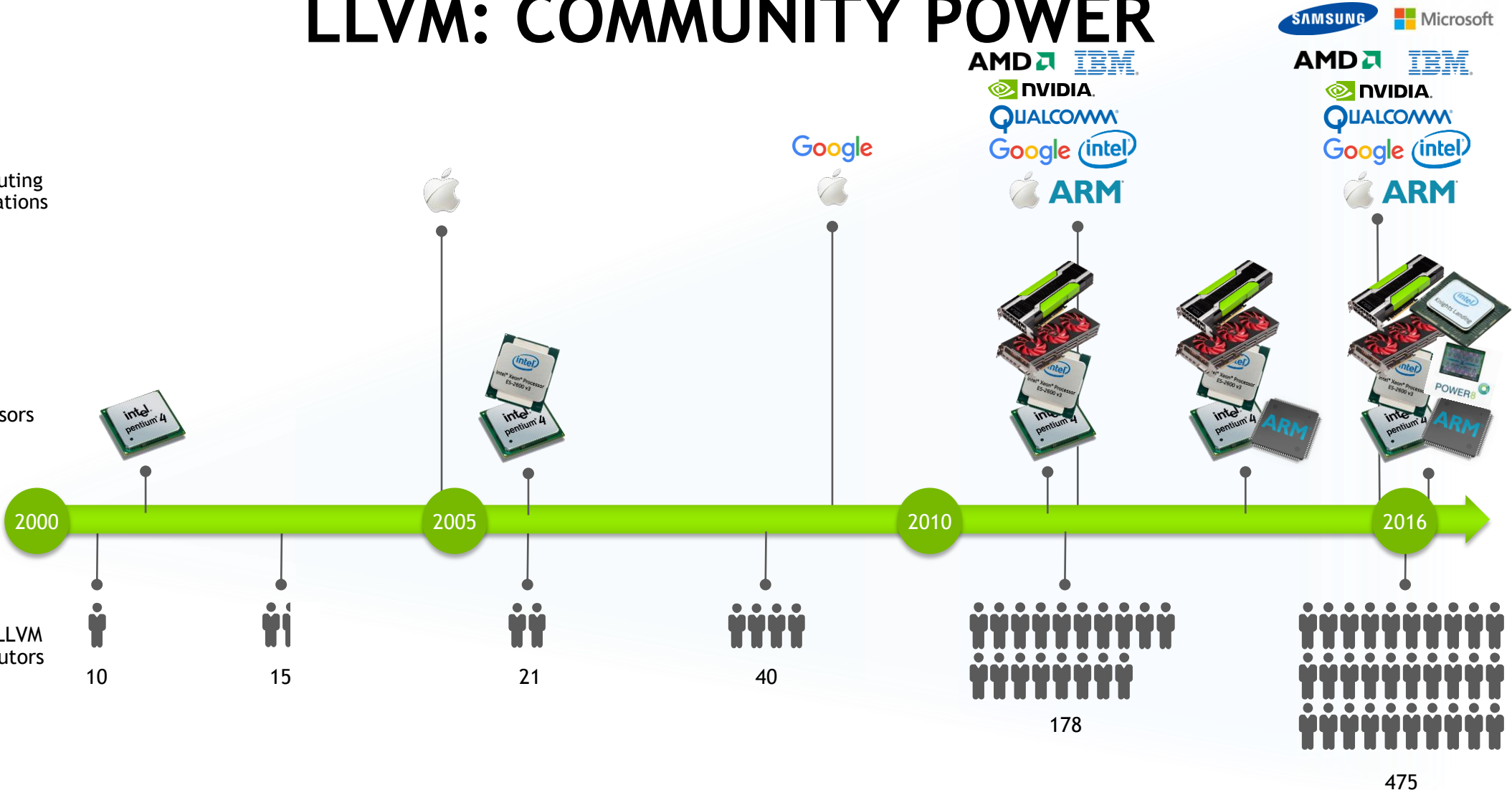
Develop CLANG-quality Fortran msg facility

LLVM: COMMUNITY POWER

Contributing Organizations

Processors

Active LLVM Contributors



AGENDA

PGI Overview

OpenACC Applications & Performance

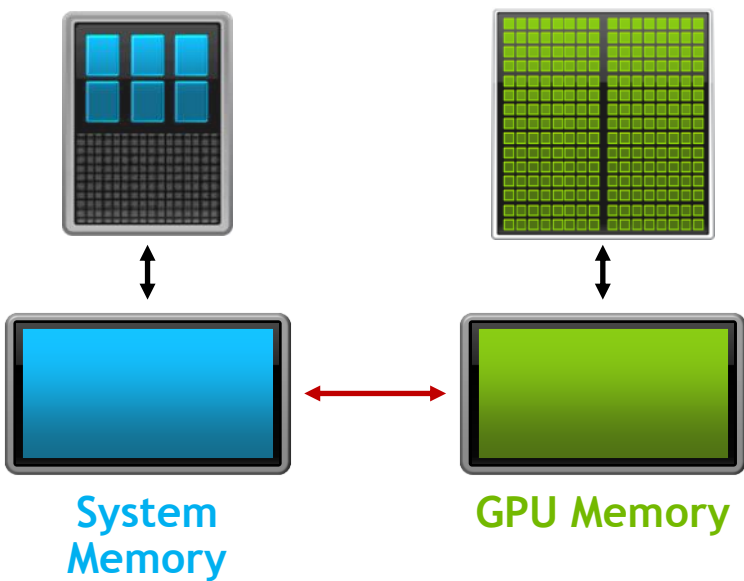
OpenPOWER & Volta V100

OpenACC and CUDA Unified Memory

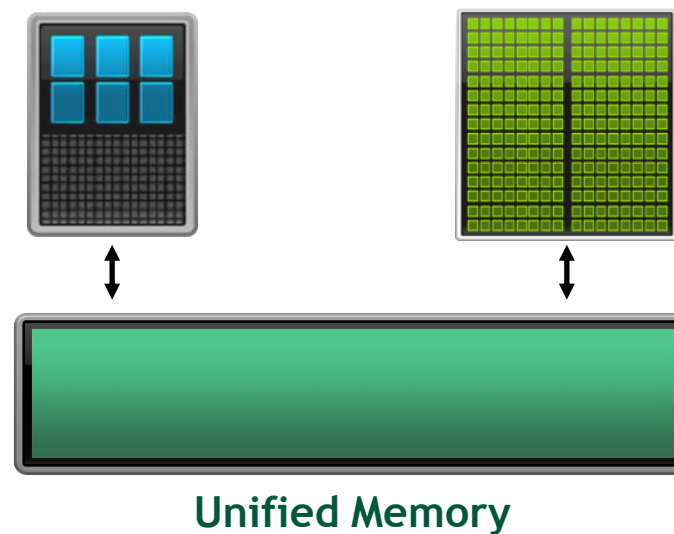
CUDA Unified Memory

Dramatically Lower Developer Effort

Developer View Today

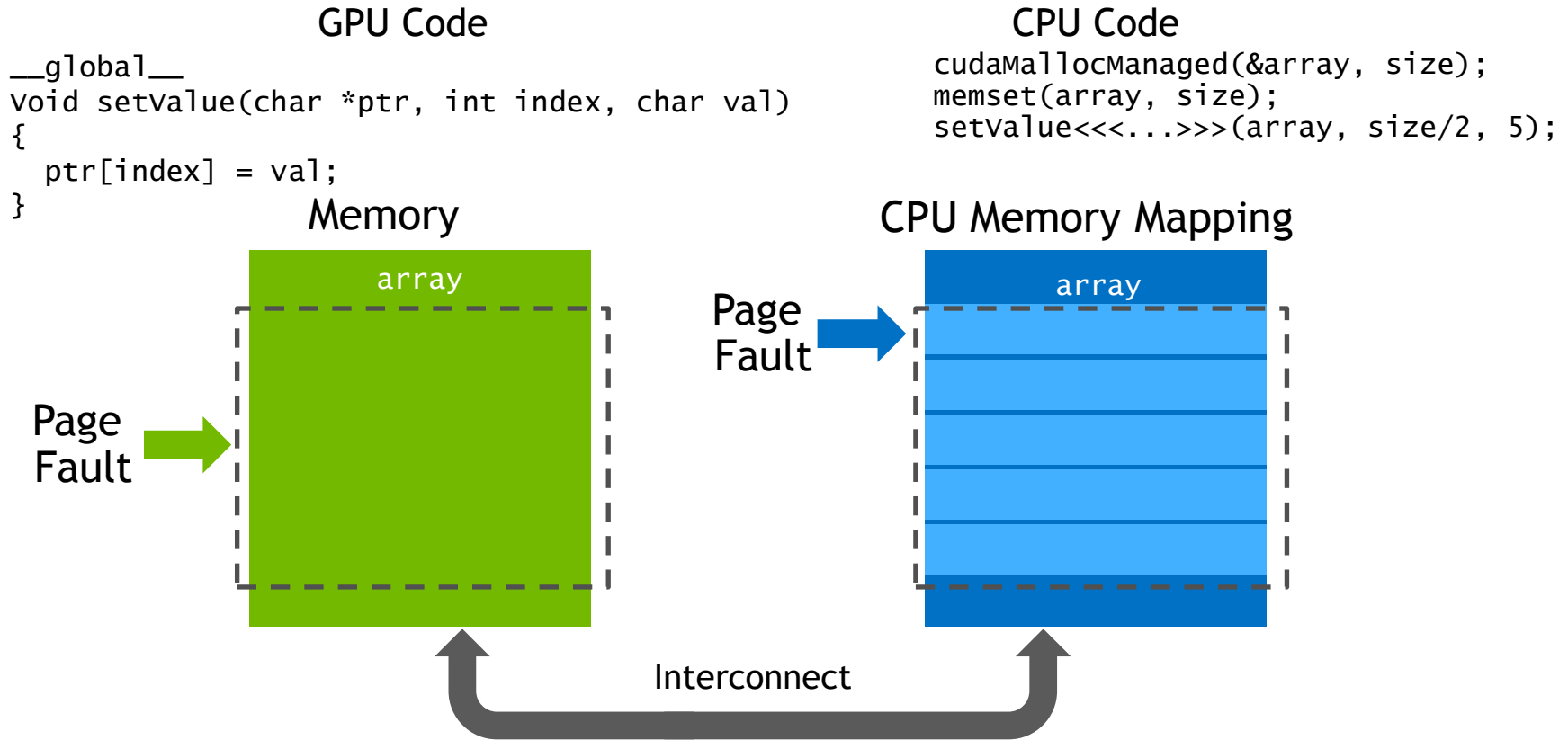


Developer View With CUDA Unified Memory



CUDA UNIFIED MEMORY ON P100

Servicing CPU *and* GPU Page Faults



OPENACC 2.6 MANUAL DEEP COPY

```
typedef struct points {  
    float* x; float* y; float* z;  
    int n;  
    float coef, direction;  
} points;
```

```
void sub ( int n, float* y ) {  
    points p;  
    #pragma acc data create (p)  
    {  
        p.n = n;  
        p.x = ( float* ) malloc ( sizeof ( float ) * n );  
        p.y = ( float* ) malloc ( sizeof ( float ) * n );  
        p.z = ( float* ) malloc ( sizeof ( float ) * n );  
        #pragma acc update device (p.n)  
        #pragma acc data copyin (p.x[0:n], p.y[0: n])  
        {  
            #pragma acc parallel loop  
            for ( i =0; i<p.n; ++I ) p.x[i] += p.y[i];  
            . . .  
        }  
    }  
}
```

DRAFT OPENACC 3.0 TRUE DEEP COPY

```
typedef struct points {
    float* x; float* y; float* z;
    int n;
    float coef, direction;
    #pragma acc policy inout(x[0:n],y[0:n])
} points;

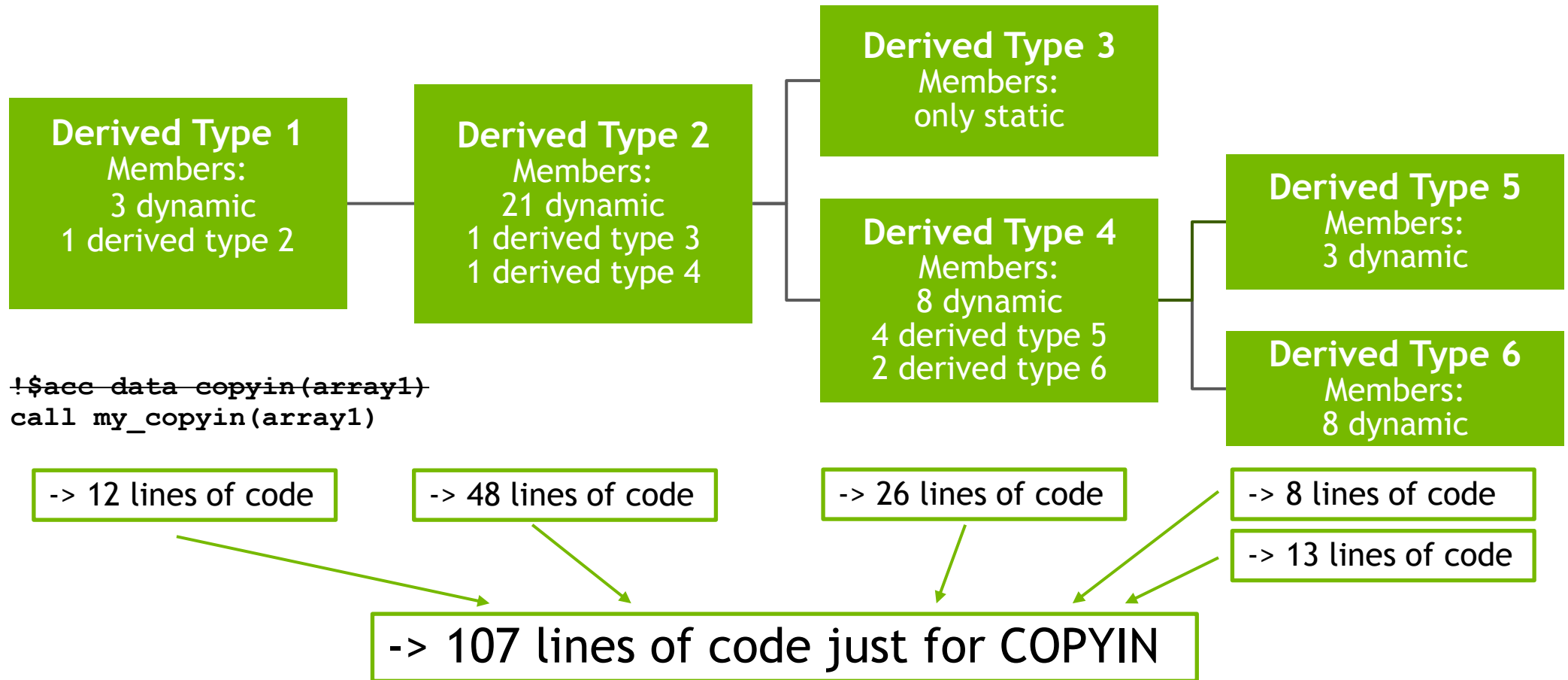
void sub ( int n, float* y ) {
    points p;

    p.n = n;
    p.x = ( float* ) malloc ( sizeof ( float ) * n );
    p.y = ( float* ) malloc ( sizeof ( float ) * n );
    p.z = ( float* ) malloc ( sizeof ( float ) * n );

    #pragma acc data copy (p)
    {
        #pragma acc parallel loop
        for ( i =0; i<p.n; ++i ) p.x[i] += p.y[i];
        . . .
    }
}
```

OPENACC 2.6 MANUAL DEEP COPY

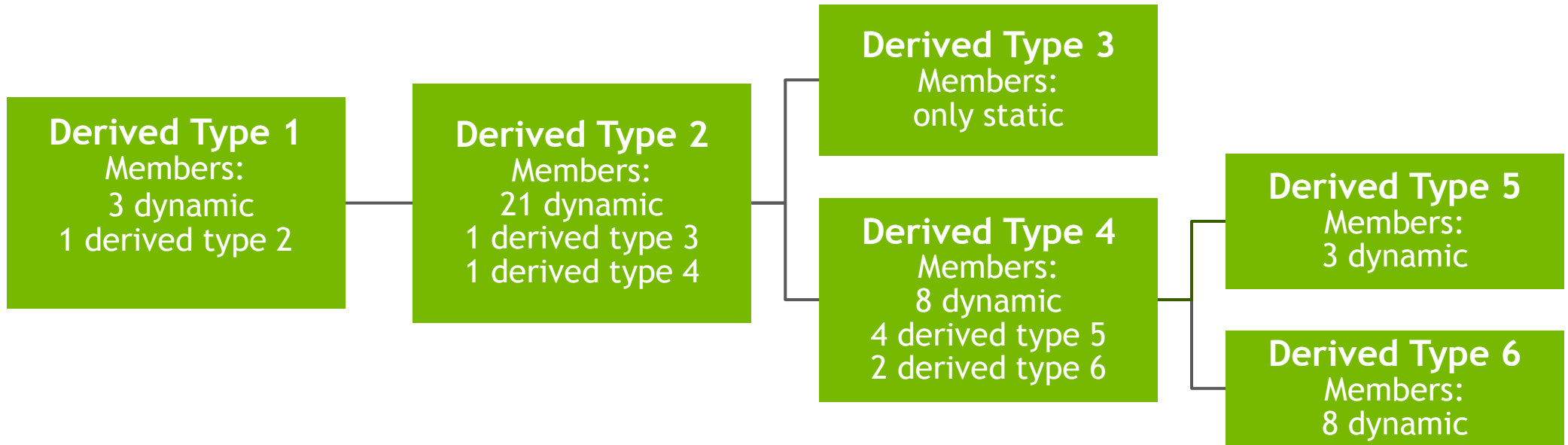
A real-world example: managing one aggregate data structure



Plus additional lines of code for COPYOUT, CREATE, UPDATE

OPENACC WITH UNIFIED MEMORY

A real-world example: managing one aggregate data structure



0 lines of code! It just works.

