# OPENACC FOR SCIENCE

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NERSC GPUs for Science Day 2019



## **OPENACC** IS...

a directives-based parallel programming model designed for usability, performance, and portability

#### Add Simple Compiler Directive

```
main()
{
    <serial code>
    #pragma acc kernels
    {
        <parallel code>
     }
}
```

## **OPENACC MEMBERS**





































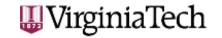












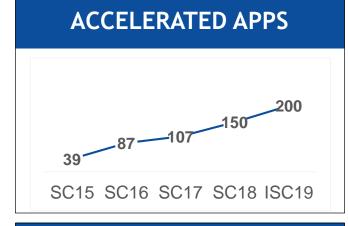


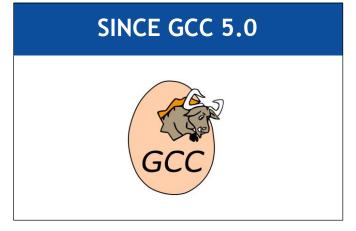


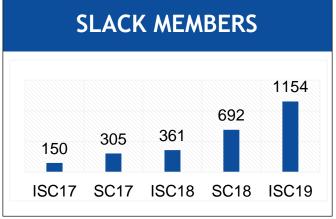
## OPENACC COMMUNITY MOMENTUM















#### **GAUSSIAN 16**



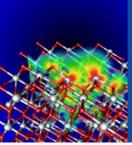
Using OpenACC allowed us to continue development of our fundamental algorithms and software capabilities simultaneously with the GPU-related work. In the end, we could use the same code base for SMP, cluster/ network and GPU parallelism. PGI's compilers were essential to the success



#### **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.



#### VASP



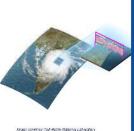
For VASP, OpenACC is the way forward for GPU acceleration. Performance is similar and in some cases better than CUDA C, and OpenACC dramatically decreases GPU development and maintenance efforts. We're excited to collaborate with NVIDIA and PGI as an early adopter of CUDA Unified Memory.



#### COSMO



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



#### E3SM



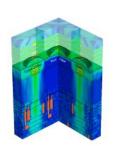
The CAAR project provided us with early access to Summit hardware and access to PGI compiler experts. Both of these were critical to our success. PGI's OpenACC support remains the best available and is competitive with much more intrusive programming



#### NUMECA FINE/Open



Porting our unstructured C++ CFD solver FINE/Open to GPUs using OpenACC would have been impossible two or three years ago, but OpenACC has developed enough that we're now getting some really good



#### SYNOPSYS



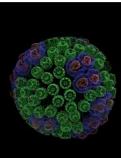
Using OpenACC, we've GPUaccelerated the Synopsys TCAD Sentaurus Device EMW simulator to speed up optical simulations of image sensors. GPUs are key to improving simulation throughput in the design of advanced image



#### MPAS-A



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.



#### **VMD**



Due to Amdahi's law, we need to port more parts of our code to the GPU if we're going to speed it up. But the sheer number of routines poses a challenge. OpenACC directives give us a low-cost approach to getting at least some speedup out of these second-tier routines. In many cases it's completely sufficient because with the current algorithms, GPU performance is bandwidth-bound.



#### **GTC**



Using OpenACC our scientists were able to achieve the acceleration needed for integrated fusion simulation with a minimum investment of time and effort in learning to program





#### **GAMERA**





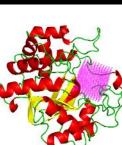






earthquake disaster simulation

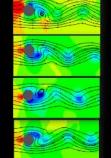
With OpenACC and a compute node based on NVIDIA's Tesla P100 GPU, we achieved more than a 14X speed up over a K Computer node running our



#### SANJEEVINI



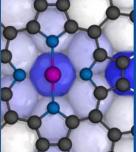
In an academic environment codes is a tedious task. OpenACC provides a great platform for computational scientists to accomplish efforts or manpower in speeding up the



#### **IBM-CFD**



OpenACC can prove to be a handy fool for CFD, we have obtained order of magnitude components of our legacy codes to GPU. Especially the routines involving search algorithm and matrix solvers have been well-accelerated to improve the overall scalability of the code



#### PWscf (Quantum ESPRESSO)





CUDA Fortran gives us the full performance potential of the CUDA programming model and NVIDIA GPUs. While leveraging the potential of explicit data movement, ISCUF KERNELS directives give us productivity and source code maintainability. It's the best



#### MAS



Adding OpenACC into MAS has given us the ability to migrate medium-sized simulations from a multi-node CPU cluster to a single multi-GPU server. The implementation yielded a portable single-source code for both CPU and GPU runs. Future work will add OpenACC to the remaining model features, enabling GPU-accelerated realistic solar storm modeling.

# INTRODUCTION TO OPENACC

# OpenACC Directives

```
Manage
              #pragma acc data copyin(a,b) copyout(c)
Data
Movement
               #pragma acc parallel
Initiate
               #pragma acc loop gang vector
Parallel
                   for (i = 0; i < n; ++i) {
Execution
                       c[i] = a[i] + b[i];
Optimize
Loop
Mappings
                                  OpenACC
```

**Directives for Accelerators** 

- Incremental
- Single source
- Interoperable
- Performance portable
- CPU, GPU, Manycore

## OPENACC SYNTAX

Syntax for using OpenACC directives in code

#### C/C++

#pragma acc directive clauses
<code>

#### Fortran

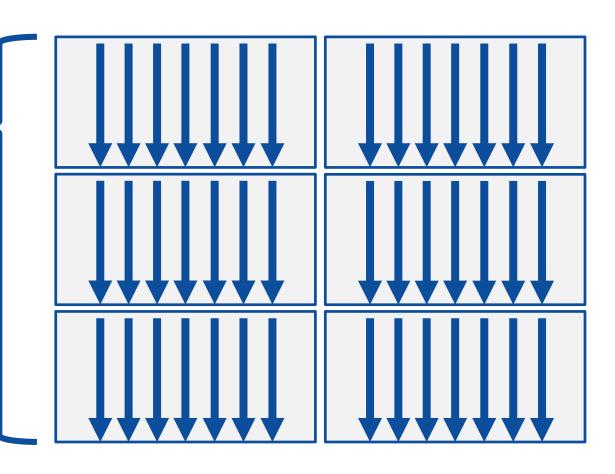
!\$acc directive clauses
<code>

- A pragma in C/C++ gives instructions to the compiler on how to compile the code.
   Compilers that do not understand a particular pragma can freely ignore it.
- A directive in Fortran is a specially formatted comment that likewise instructions the compiler in it compilation of the code and can be freely ignored.
- "acc" informs the compiler that what will come is an OpenACC directive
- Directives are commands in OpenACC for altering our code.
- Clauses are specifiers or additions to directives.

## OPENACC PARALLEL LOOP DIRECTIVE

Expressing parallelism

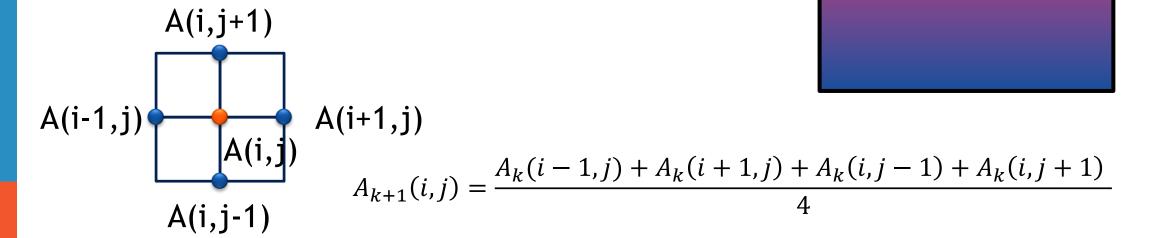
```
#pragma acc parallel loop
   for(int i = 0; i < N; i++)</pre>
       // Do Something
    Generate parallelism and
     parallelize the next loop
                nest
```



## OPENACC EXAMPLE

## **EXAMPLE: JACOBI ITERATION**

- Iteratively converges to correct value (e.g. Temperature), by computing new values at each point from the average of neighboring points.
- Common, useful algorithm
- Example: Solve Laplace equation in 2D:  $\nabla^2 f(x, y) = 0$



## JACOBI ITERATION: C CODE

```
while ( err > tol && iter < iter max ) {</pre>
  err=0.0;
  for ( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {
      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                            A[j-1][i] + A[j+1][i]);
      err = max(err, abs(Anew[j][i] - A[j][i]));
  for ( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
  iter++;
```

Iterate until converged

Iterate across matrix elements

Calculate new value from neighbors

Compute max error for convergence

Swap input/output arrays

### PARALLELIZE WITH OPENACC PARALLEL LOOP

```
while ( err > tol && iter < iter max ) {</pre>
  err=0.0;
#pragma acc parallel loop reduction(max:err)
  for ( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {
      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);
      err = max(err, abs(Anew[j][i] - A[j][i]));
#pragma acc parallel loop
  for( int j = 1; j < n-1; j++) {
    for ( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
  iter++;
```

Parallelize first loop nest, max *reduction* required.

Parallelize second loop.

We didn't detail how to parallelize the loops, just which loops to parallelize.

# BUILDING THE CODE (GPU)

```
$ pgcc -fast -ta=tesla:managed -Minfo=accel laplace2d uvm.c
main:
     63, Accelerator kernel generated
         Generating Tesla code
         64, #pragma acc loop gang /* blockIdx.x */
             Generating reduction(max:error)
         66, #pragma acc loop vector(128) /* threadIdx.x */
     63, Generating implicit copyin(A[:])
         Generating implicit copyout(Anew[:])
         Generating implicit copy(error)
     66, Loop is parallelizable
     74, Accelerator kernel generated
         Generating Tesla code
         75, #pragma acc loop gang /* blockIdx.x */
         77, #pragma acc loop vector(128) /* threadIdx.x */
     74, Generating implicit copyin(Anew[:])
         Generating implicit copyout(A[:])
     77, Loop is parallelizable
```

Instruct the compiler to build for an NVIDIA Tesla GPU using "CUDA Managed Memory"\*

Print compiler feedback so we can see what it did.

<sup>\*</sup> More on this in a moment

# BUILDING THE CODE (GPU)

```
$ pgcc -fast -ta=tesla:managed -Minfo=accel laplace2d uvm.c
main:
     63, Accelerator kernel generated
         Generating Tesla code
         64, #pragma acc loop gang /* blockIdx.x */
             Generating reduction(max:error)
         66, #pragma acc loop vector(128) /* threadIdx.x */
     63, Generating implicit copyin(A[:])
         Generating implicit copyout(Anew[:])
                                                                 Affirms that a GPU kernel
         Generating implicit copy(error)
     66, Loop is parallelizable
                                                                     was generated.
     74, Accelerator kernel generated
         Generating Tesla code
         75, #pragma acc loop gang /* blockIdx.x */
                                                                    Compiler detected
         77, #pragma acc loop vector(128) /* threadIdx.x */
                                                                  possible need to move
     74, Generating implicit copyin(Anew[:])
         Generating implicit copyout(A[:])
                                                                  data and handled it for
     77, Loop is parallelizable
                                                                           us.*
```

<sup>\*</sup> More on this in a moment

# BUILDING THE CODE (MULTICORE)

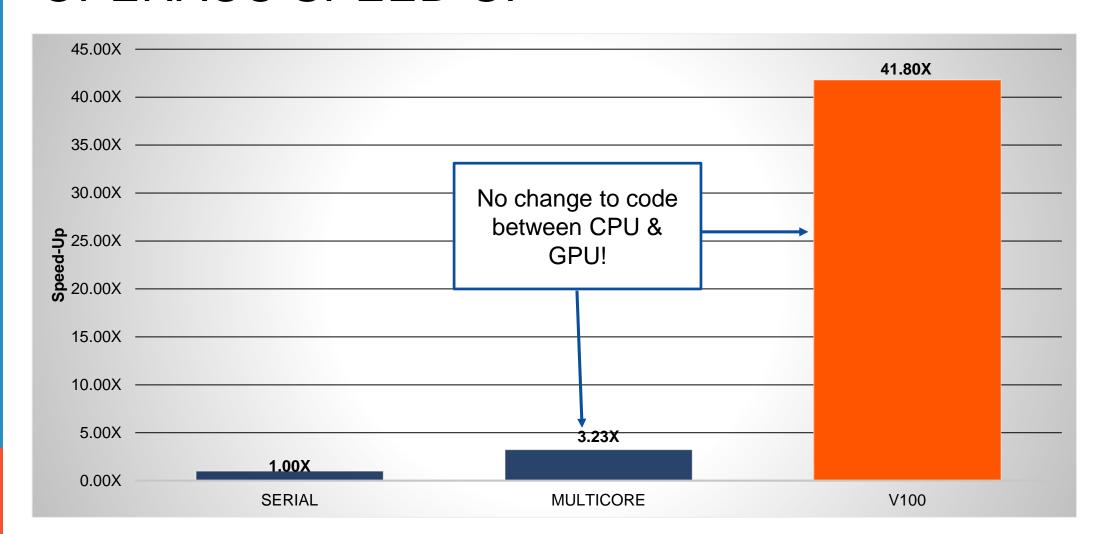
```
$ pgcc -fast -ta=multicore -Minfo=accel laplace2d_uvm.c

main:

63, Generating Multicore code
64, #pragma acc loop gang
64, Accelerator restriction: size of the GPU copy of Anew,
Generating reduction(max:error)
66, Loop is parallelizable
74, Generating Multicore code
75, #pragma acc loop gang
75, Accelerator restriction: size of the GPU copy of Anew, A is unknown
77, Loop is parallelizable
```

Building for a multicore CPU requires changing only a compiler flag.

## **OPENACC SPEED-UP**

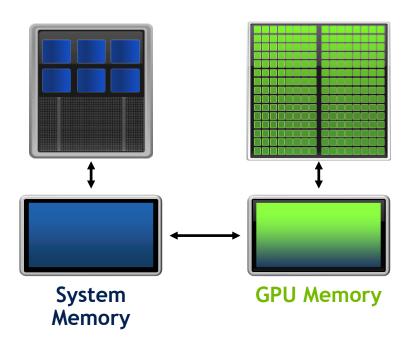


## CUDA UNIFIED MEMORY

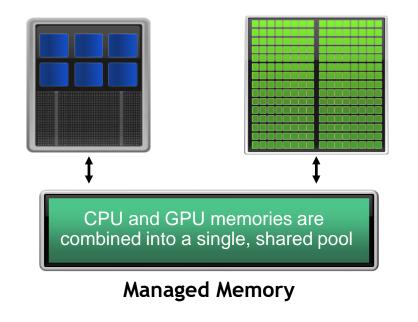
Simplified Developer Effort

Commonly referred to as "managed memory."

#### Without Managed Memory



#### With Managed Memory



## CUDA MANAGED MEMORY

- Handling explicit data transfers between the host and device (CPU and GPU) can be difficult
- The PGI compiler can utilize CUDA Managed Memory to defer data management
- This allows the developer to concentrate on parallelism and think about data movement as an optimization
- But, the programmer can usually do better by explicitly managing the data movement.

```
$ pgcc -fast -acc -ta=tesla:managed -Minfo=accel main.c
```

```
$ pgfortran -fast -acc -ta=tesla:managed -Minfo=accel main.f90
```

## BUILDING THE CODE (W/O MANAGED MEMORY)

```
$ pgcc -fast -ta=tesla -Minfo=accel laplace2d uvm.c
PGC-S-0155-Compiler failed to translate accelerator region (see -Minfo messages):
Could not find allocated-variable index for symbol (laplace2d uvm.c: 63)
PGC-S-0155-Compiler failed to translate accelerator region (see -Minfo messages):
Could not find allocated-variable index for symbol (laplace2d uvm.c: 74)
main:
     63, Accelerator kernel generated
         Generating Tesla code
         63, Generating reduction (max:error)
         64, #pragma acc loop gang /* blockIdx.x */
         66, #pragma acc loop vector(128) /* threadIdx.x */
     64, Accelerator restriction: size of the GPU copy of Anew, A is unknown
     66, Loop is parallelizable
     74, Accelerator kernel generated
         Generating Tesla code
         75, #pragma acc loop gang /* blockIdx.x */
         77, #pragma acc loop vector(128) /* threadIdx.x */
     75, Accelerator restriction: size of the GPU copy of Anew, A is unknown
     77, Loop is parallelizable
```

\* "managed" keyword removed from tesla target, fails to build

## OPENACC DATA MANAGEMENT

## OPENACC DATA DIRECTIVE

#### **Definition**

- The data directive defines a lifetime for data on the device
- During the region data should be treated as owned by the accelerator
- Data clauses allow the programmer to control the allocation and movement of data
- When memory is shared, regions may be ignored

```
#pragma acc data clauses
{
     < Sequential and/or Parallel code >
}
```

```
!$acc data clauses
  < Sequential and/or Parallel code >
!$acc end data
```

## DATA CLAUSES

Copy ( list ) Allocates memory on GPU and copies data from host to GPU when entering region and copies data to the host when exiting region.

Principal use: For many important data structures in your code, this is a logical default to input, modify and return the data.

copyin ( list ) Allocates memory on GPU and copies data from host to GPU when entering region.

Principal use: Think of this like an array that you would use as just an input to a subroutine.

copyout ( list ) Allocates memory on GPU and copies data to the host when exiting region.

Principal use: A result that isn't overwriting the input data structure.

create ( list ) Allocates memory on GPU but does not copy.

Principal use: Temporary arrays.

## ARRAY SHAPING

- Sometimes the compiler needs help understanding the shape of an array
- The first number is the start index of the array
- In C/C++, the second number is how much data is to be transferred
- In Fortran, the second number is the ending index

```
copy(array[starting_index:length])
```

C/C++

copy(array(starting\_index:ending\_index))

**Fortran** 

### OPTIMIZED DATA MOVEMENT

```
#pragma acc data copy(A[:n*m]) create(Anew[:n*m])
while ( err > tol && iter < iter max ) {</pre>
  err=0.0;
#pragma acc parallel loop reduction(max:err)
  for ( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {
      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);
      err = max(err, abs(Anew[j][i] - A[j][i]));
#pragma acc parallel loop
  for ( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
  iter++;
```

Copy A to/from the accelerator only when needed.

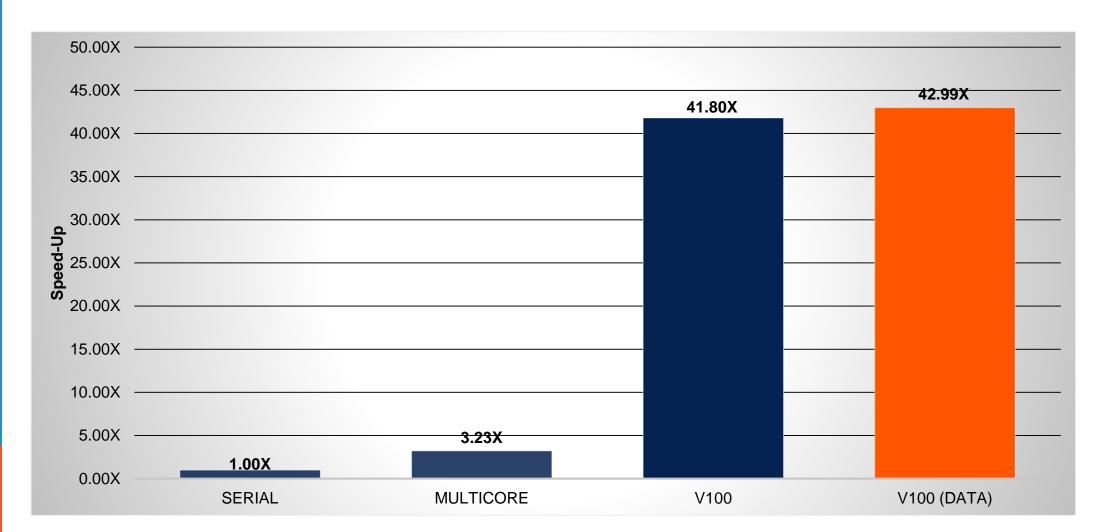
Create temporary space for Anew

#### REBUILD THE CODE

```
pgcc -fast -ta=tesla -Minfo=accel laplace2d uvm.c
main:
     60, Generating copy(A[:m*n])
         Generating copyin (Anew[:m*n])
     64, Accelerator kernel generated
         Generating Tesla code
         64, Generating reduction (max:error)
         65, #pragma acc loop gang /* blockIdx.x */
         67, #pragma acc loop vector(128) /* threadIdx.x */
     67, Loop is parallelizable
     75, Accelerator kernel generated
         Generating Tesla code
         76, #pragma acc loop gang /* blockIdx.x */
         78, #pragma acc loop vector(128) /* threadIdx.x */
     78, Loop is parallelizable
```

Now data movement only happens at our data region.

## **OPENACC SPEED-UP**



# OPENACC CASE STUDIES

## OPENACC CASE STUDIES

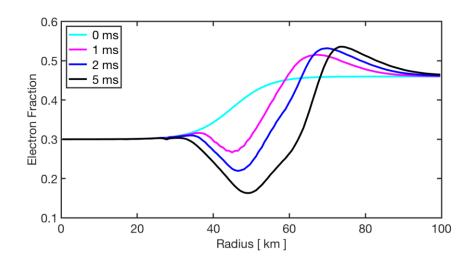
#### Real life lessons learned

- Thornado: OpenACC Interoperability with math libraries (Collaboration with Austin Harris, ORNL)
- E3SM: OpenACC with Unified Memory for Fortran Derived Types (Collaboration with Matt Norman, ORNL)

# THORNADO

## THORNADO – NEUTRINO TRANSPORT

- Neutrino transport problem mimicking core-collapse supernova
- DG-IMEX scheme
- Energy discretization: 32 points with  $\varepsilon \in [0,300]$  MeV
- Spatial discretization:  $12^3$  points with  $(x, y, z) \in [0,100]$
- Deleptonization Wave test
- Mock initial CCSN profile
- Initial neutrino spectrum from Fermi-Dirac distribution



## GPU CODE TRANSFORMATION EXAMPLE

#### **Original CPU code**

DO i6=1,n5; ...; DO i2=1,n2

! Calculate G(:,i2,i3,i4,i5,i6)

DO i1=1,n1

! Calculate V(:,i1,i2,i3,i4,i5,i6)

! Calculate S(:,i1,i2,i3,i4,i5,i6)

! Calculate U(:,i1,i2,i3,i4,i5,i6)

**END DO** 

END DO; ...; END DO

#### OpenACC code

! Calculate G 8 DGEMM

**8 DGEMV** ! Calculate S **2 DGEMM** 

!\$ACC PARALLEL LOOP GANG VECTOR COLLAPSE(7)

DO i6=1,n6; ...; DO i0=1,n0

**8 DGEMV** ! Calculate V(i0,i1,i2,i3,i4,i5,i6)

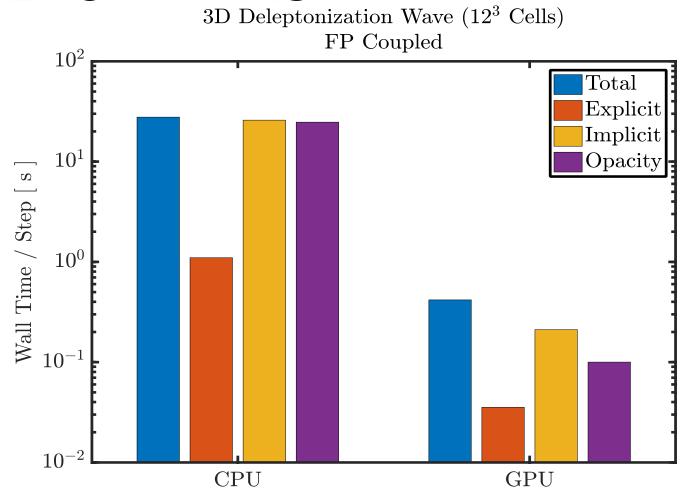
**12 DGEMV** END DO; ...; END DO

! Calculate U 3 DGEMM

# OPENACC/CUBLAS INTEROPERABILITY (DNRM2)

```
MODULE LinearAlgebraModule
USE DeviceModule
                                                                                MODULE OpenACCModule
SUBROUTINE VectorNorm2( n, x, incx, xnorm )
REAL(8), DIMENSION(:), POINTER :: px
                                                                                INTEGER(C INT) FUNCTION acc is present(hostptr,bytes) &
                                                                                 BIND(C,NAME="acc is present")
                     :: hx, dx
TYPE(C PTR)
                    :: data on device
                                                                                USE, INTRINSIC:: iso c binding
LOGICAL
                                                                                TYPE(C PTR), VALUE :: hostptr
data on device = .false.
size of x = n * c size of(0.0d0)
                                                                                INTEGER(C SIZE T), VALUE :: bytes
px(1:n) => x(1:n)
                                                                                END FUNCTION
hx = C LOC(px)
data on device = device is present( hx, mydevice, size of x )
IF (data on device) THEN
                                                                                MODULE DeviceModule
#if defined(THORNADO OACC)
                                                                                USE OpenACCModule
!$ACC HOST DATA USE DEVICE( px )
                                                                                LOGICAL FUNCTION device is present (hostptr, device, bytes)
#endif
                                                                                TYPE(C PTR), INTENT(in) :: hostptr
dx = C LOC(px)
                                                                                INTEGER, INTENT(in) :: device
#if defined(THORNADO OACC)
                                                                                INTEGER(C SIZE T), INTENT(in) :: bytes
!$ACC END HOST DATA
                                                                                #if defined(THORNADO OACC)
#endif
                                                                                device is present = ( acc is present( hostptr, bytes ) > 0 )
ierr = cublasDnrm2 v2( cublas handle, n, dx, incx, xnorm )
                                                                                #else
ELSE
                                                                                device is present = .false.
xnorm = DNRM2(n, x, incx)
                                                                                #endif
END IF
                                                                                END FUNCTION
END SUBROUTINE
```

## **GPU BENCHMARKS**



## PROGRAMMING MODEL COMPARISON

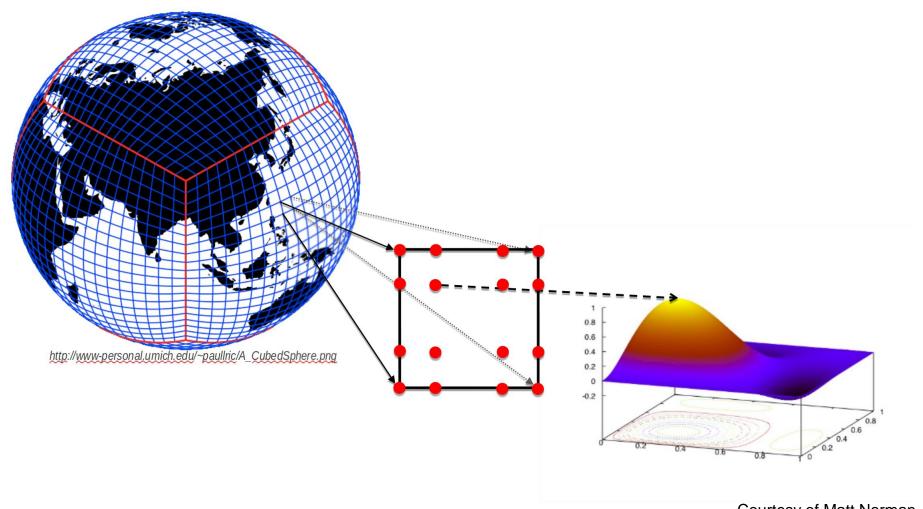
Compiler	Offload Model	$T_CPU$	$T_GPU$	Speedup
PGI v19.4	OpenACC v2.7	27.8 sec/step	0.42 sec/step	67X
XL v16.1.1	OpenMP v4.5	25.6 sec/step	0.99 sec/step	26X

# E3SM

# The Energy Exascale Earth System Model (E3SM)

- The U.S. DOE's high-resolution climate model
- Coupling of five components: (1) Atmosphere, (2) Ocean, (3)
   Land Surface, (4) Sea Ice, and (5) Land Ice
- Atmospheric model is most expensive component
  - "Cubed-sphere" non-orthogonal grid
  - Spectral Element method (continuous Galerkin, timeexplicit)
- Because of throughput requirements, hi-res climate has very little work per node to accelerate

# The Energy Exascale Earth System Model (E3SM)



## COMPLEX DATA TYPES

```
type crm_rad_type
17
18
         ! Radiative heating
         real(crm rknd), pointer :: qrad(:,:,:,:)
19
20
21
         ! Quantities used by the radiation code. Note that these are strange in that they are
22
         ! time-averages, but spatially-resolved.
23
         real(crm rknd), pointer :: temperature(:,:,:) ! rad temperature
         real(crm_rknd), pointer :: qv (:,:,:) ! rad vapor
24
         real(crm_rknd), pointer :: qc (:,:,:,:) ! rad cloud water
25
         real(crm_rknd), pointer :: qi (:,:,:) ! rad cloud ice
26
27
         real(crm rknd), pointer :: cld(:,:,:,:) ! rad cloud fraction
28
29
         ! Only relevant when using 2-moment microphysics
         real(crm_rknd), pointer :: nc(:,:,:) ! rad cloud droplet number (#/kg)
30
31
         real(crm rknd), pointer :: ni(:,:,:) ! rad cloud ice crystal number (#/kg)
         real(crm_rknd), pointer :: qs(:,:,:) ! rad cloud snow (kg/kg)
32
33
         real(crm rknd), pointer :: ns(:,:,:) ! rad cloud snow crystal number (#/kg)
34
     end type crm rad type
```

Using the managed memory option enabled this GPU port.

## USING CUDA PREFETCH HINTS

Interface with CUDA prefetch API to improve performance

```
119
     subroutine memset_r8_flat(a,n,v,asyncid)
120
       implicit none
121 real(8) :: a(n)
122 real(8) :: v
123 integer :: n, asyncid, i
124 #if defined( OPENACC) && defined ( CUDA)
125 !$acc host data use device(a)
126 ierr = cudaMemsetAsync( a , v , n , acc_get_cuda_stream(asyncid) )
127
       !$acc end host data
128 #else
129
       !$acc parallel loop async(asyncid)
130
       do i=1,n
131 \qquad a(i) = v
132 enddo
133 #endif
134 end subroutine memset r8 flat
```

## PREFETCH WRAPPERS

Examples of multi-dimension pre-fectch

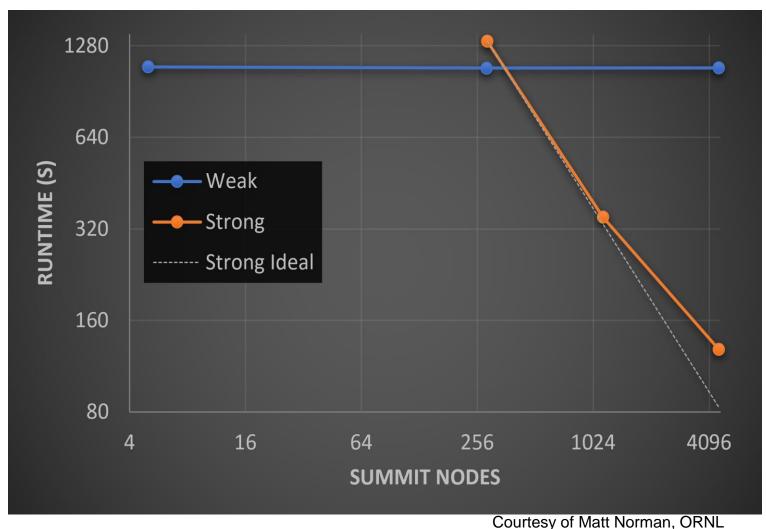
```
subroutine prefetch_r8_3d(a)
                                  553
                                  554
                                            implicit none
                                            real(8) :: a(:,:,:)
                                  555
    subroutine prefetch r8 flat(a,n)
203
                                            call prefetch_r8_flat(a,product(shape(a)))
                                  556
204
      implicit none
205
                                         end subroutine prefetch r8 3d
      real(8) :: a(n)
                                  557
206
      integer :: n
207 #if defined( OPENACC) && defined ( CUDA)
208
      !$acc host data use device(a)
209
      ierr = cudaMemPrefetchAsync( a , n , acc_get_device_num(acc_device_nvidia) , acc_get_cuda_stream(asyncid_loc+1) ]
210
      !$acc end host data
211 #endif
                 subroutine memset r8 3d(a,v,asyncid)
    end s 316
         317
                   implicit none
                   real(8) :: a(:,:,:)
         318
                   real(8) :: v
         319
         320
                   integer :: asyncid
                   call memset_r8_flat(a,product(shape(a)),v,asyncid)
         321
                end subroutine memset r8 3d
         322
```

# Performance on OLCF Summit Supercomputer

Runtime for one model day

Weak: 28km GCM with 64x64 columns per CRM

Strong: 28km GCM with 16x16 columns per CRM



# Performance on OLCF Summit Supercomputer

- Gordon Bell simulations: 3-D 500m global grid spacing at 2 SYPD
  - 28km GCM grid spacing, 64x64 CRM columns per GCM column
  - Using 4,600 nodes of Summit, we get 2.5% peak flop/s
  - 2.5% peak flops on Volta GPU = 33 flops per memory load / store
  - About 200 kernels in 30K LOCs using PGI OpenACC
- Current <u>production</u> simulations: 2-D CRM at 500m dx at 3 SYPD
  - 3 SYPD with 28km GCM grid spacing and 64x1 columns per CRM
  - Using 1,000 Summit nodes, also 2.5% peak flop/s
  - About 15x speed-up using 6 Voltas/node versus 2 Power9/node

# CLOSING

## CONCLUSION

OpenACC is a mature, directive-based programming model that is available for GPUs, multicore CPUs, and more and is in use by more than 200 scientific applications.

## OPENACC RESOURCES

Guides • Talks • Tutorials • Videos • Books • Spec • Code Samples • Teaching Materials • Events • Success Stories • Courses • Slack • Stack Overflow



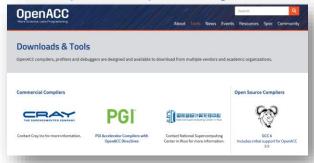
#### Resources

https://www.openacc.org/resources



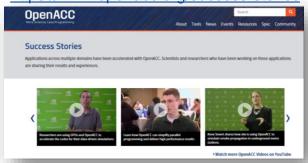
#### **Compilers and Tools**

https://www.openacc.org/tools



#### **Success Stories**

https://www.openacc.org/success-stories



#### **Events**

https://www.openacc.org/events

