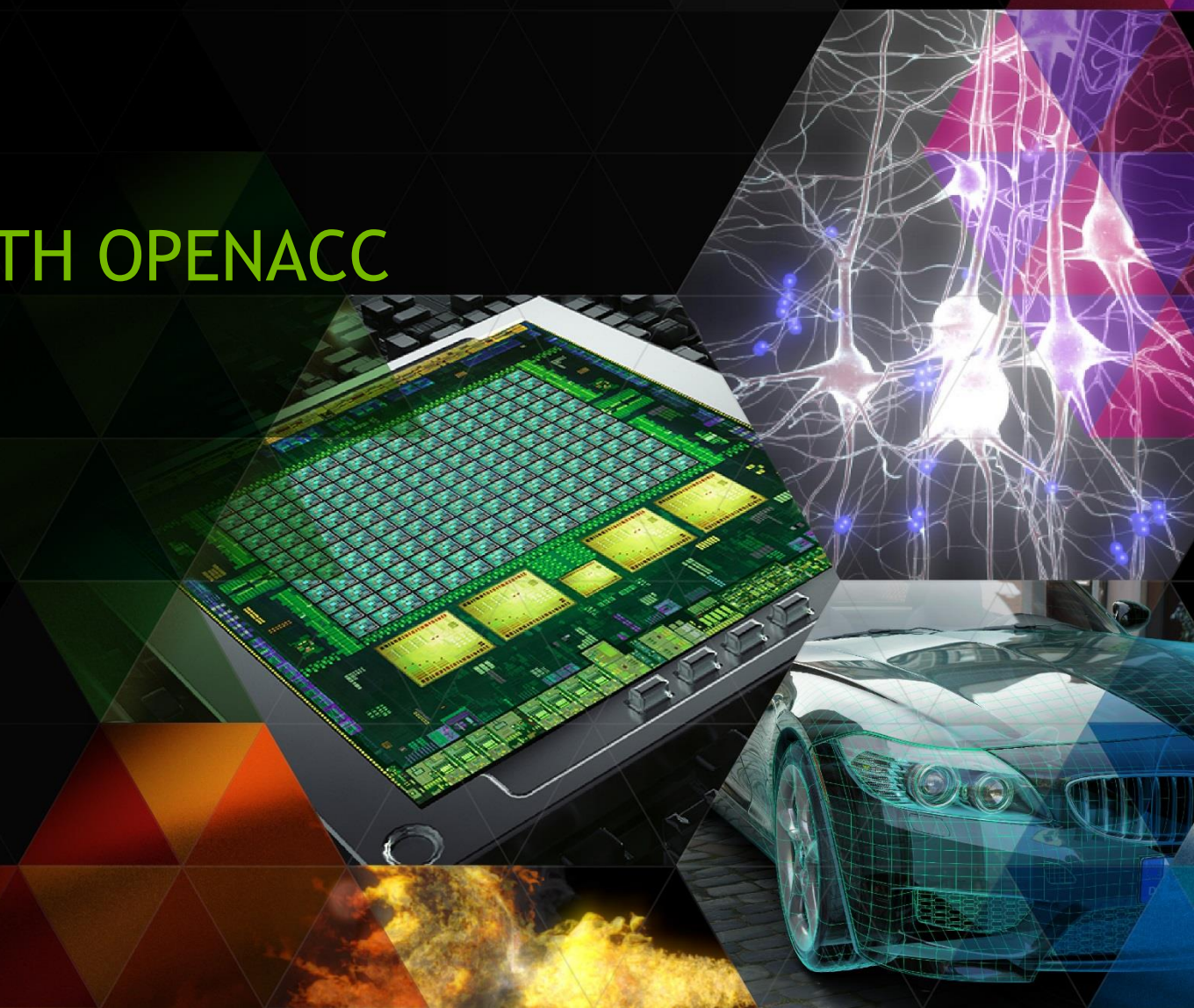
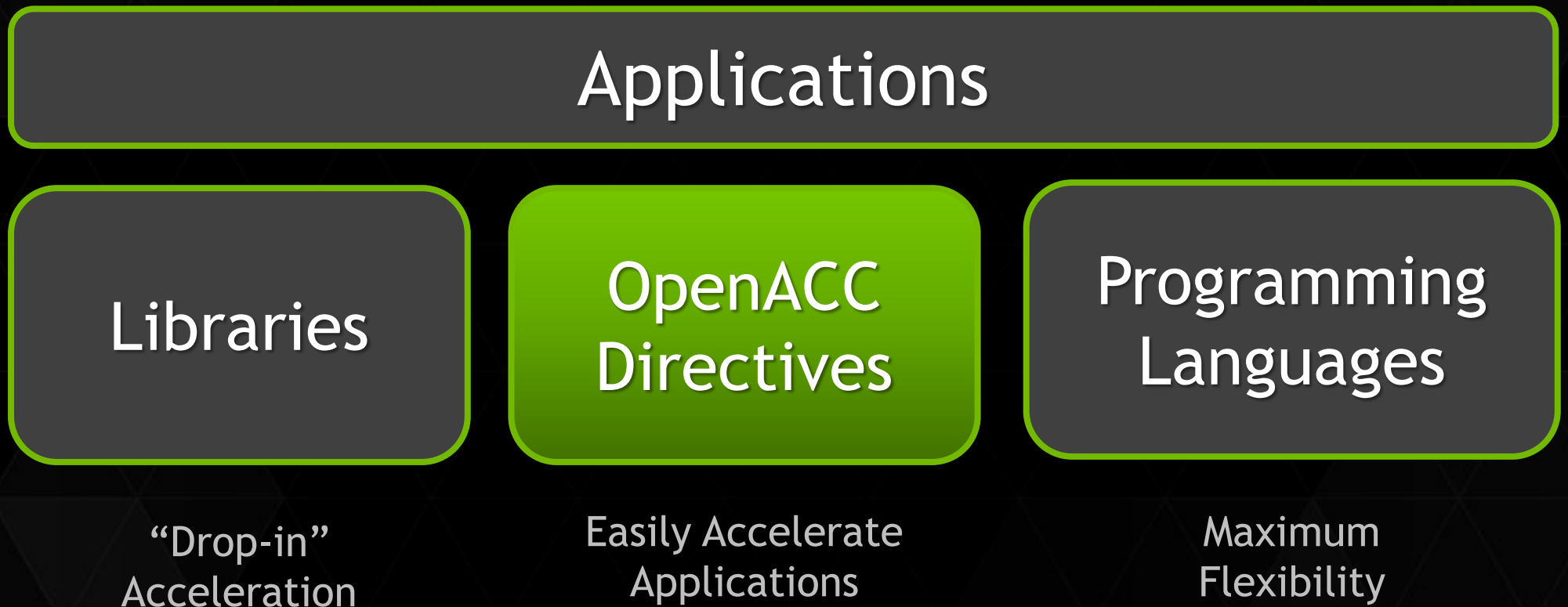
NVIDIA

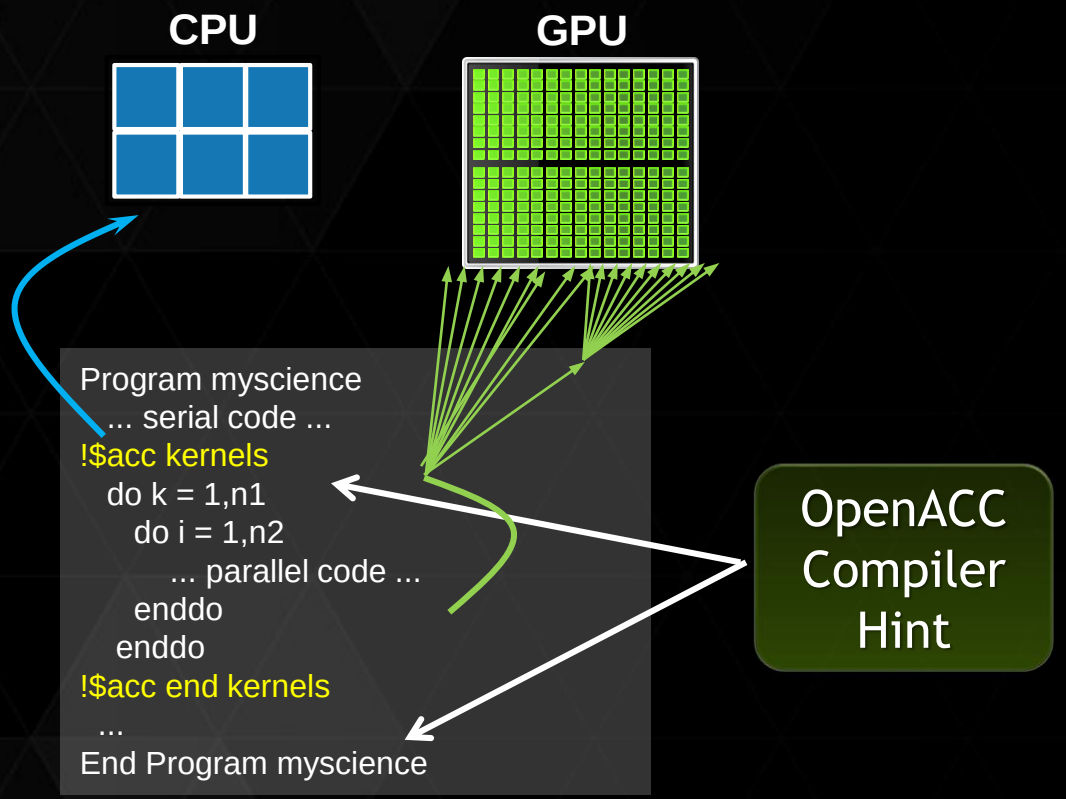
GPU COMPUTING WITH OPENACC



3 WAYS TO ACCELERATE APPLICATIONS



OPENACC DIRECTIVES



Your original Fortran or C code

Simple Compiler hints

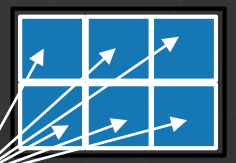
Compiler Parallelizes code

Works on many-core GPUs & multicore CPUs

FAMILIAR TO OPENMP PROGRAMMERS

OpenMP

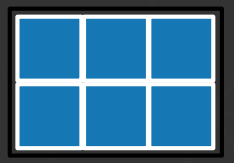
CPU



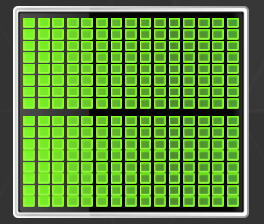
```
main() {
  double pi = 0.0; long i;

  #pragma omp parallel for reduction(+:pi)
  for (i=0; i<N; i++)
  {
    double t = (double)((i+0.05)/N);
    pi += 4.0/(1.0+t*t);
  }

  printf("pi = %f\n", pi/N);
}
```

OpenACC

CPU



GPU



```
main() {
  double pi = 0.0; long i;

  #pragma acc kernels
  for (i=0; i<N; i++)
  {
    double t = (double)((i+0.05)/N);
    pi += 4.0/(1.0+t*t);
  }

printf("pi = %f\n", pi/N);
}
```

OpenACC Members and Supporters

DIRECTIVES: EASY & POWERFUL

Real-Time Object Detection

Global Manufacturer of Navigation Systems

5x in 40 Hours

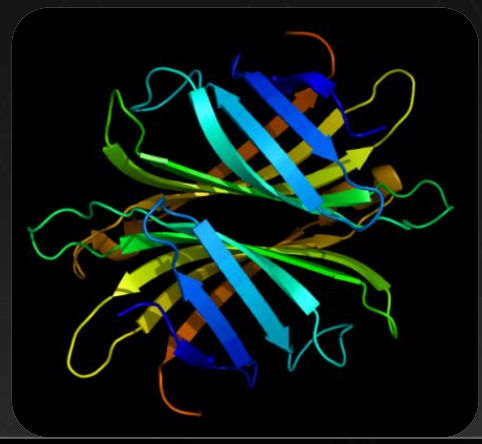
Valuation of Stock Portfolios using Monte Carlo

Global Technology Consulting Company

2x in 4 Hours

Interaction of Solvents and Biomolecules

University of Texas at San Antonio



5x in 8 Hours

"Optimizing code with directives is quite easy, especially compared to CPU threads or writing CUDA kernels. The most important thing is avoiding restructuring of existing code for production applications."

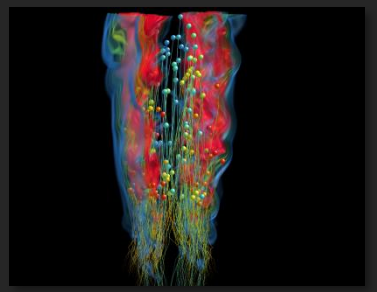
-- Developer at the Global Manufacturer of Navigation Systems

FOCUS ON EXPOSING PARALLELISM

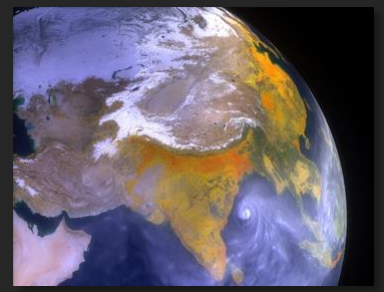
With Directives, tuning work focuses on *exposing parallelism*, which makes codes inherently better

Example: Application tuning work using directives for new Titan system at ORNL

S3D
Research more efficient combustion with next-generation fuels



- **Tuning top 3 kernels (90% of runtime)**
- ***3 to 6x faster on CPU+GPU vs. CPU+CPU***
- **But also improved all-CPU version by 50%**



CAM-SE
Answer questions about specific climate change adaptation and mitigation scenarios

- **Tuning top key kernel (50% of runtime)**
- **6.5x faster on CPU+GPU vs. CPU+CPU**
- **Improved performance of CPU version by 100%**

A VERY SIMPLE EXERCISE: SAXPY

SAXPY in C

```
void saxpy(int n,
           float a,
           float *x,
           float *restrict y)
{
#pragma acc kernels
  for (int i = 0; i < n; ++i)
    y[i] = a*x[i] + y[i];
}

...
// Perform SAXPY on 1M elements
saxpy(1<<20, 2.0, x, y);
...
```

SAXPY in Fortran

```
subroutine saxpy(n, a, x, y)
  real :: x(:), y(:), a
  integer :: n, i
$!acc kernels
  do i=1,n
    y(i) = a*x(i)+y(i)
  enddo
$!acc end kernels
end subroutine saxpy


...
$ Perform SAXPY on 1M elements
call saxpy(2**20, 2.0, x_d, y_d)
...
```

DIRECTIVE SYNTAX

- Fortran

  ```
  !$acc directive [clause [,] clause] …]
  ```

  Often paired with a matching end directive surrounding a structured code block

  ```
  !$acc end directive
  ```

- C

  ```
  #pragma acc directive [clause [,] clause] …]
  ```

  Often followed by a structured code block

KERNELS: YOUR FIRST OPENACC DIRECTIVE

Each loop executed as a separate *kernel* on the GPU.

```
!$acc kernels
    do i=1,n
       a(i) = 0.0
       b(i) = 1.0
       c(i) = 2.0
    end do

    do i=1,n
       a(i) = b(i) + c(i)
    end do
!$acc end kernels
```

kernel 1

kernel 2

Kernel:
A parallel function that runs on the GPU

KERNELS CONSTRUCT

Fortran

```
!$acc kernels [clause …]
    structured block
!$acc end kernels
```

C

```
#pragma acc kernels [clause …]
    { structured block }
```

Clauses

```
if( condition )

async( expression )
```

Also, any data clause (more later)

COMPLETE SAXPY EXAMPLE CODE

- Trivial first example
  - Apply a loop directive
  - Learn compiler commands

```
#include <stdlib.h>

void saxpy(int n,
           float a,
           float *x,
           float *restrict y)
{
#pragma acc kernels
for (int i = 0; i < n; ++i)
    y[i] = a * x[i] + y[i];
}
```

*restrict:
"I promise y does not alias x"

```
int main(int argc, char **argv)
{
  int N = 1<<20; // 1 million floats

  if (argc > 1)
    N = atoi(argv[1]);

  float *x = (float*)malloc(N * sizeof(float));
  float *y = (float*)malloc(N * sizeof(float));

  for (int i = 0; i < N; ++i) {
    x[i] = 2.0f;
    y[i] = 1.0f;
  }

  saxpy(N, 3.0f, x, y);

  return 0;
}
```

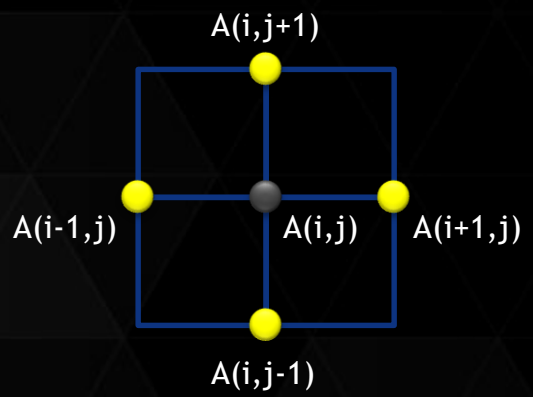
COMPILE AND RUN

- C: **`pgcc -acc -ta=nvidia -Minfo=accel -o saxpy_acc saxpy.c`**
- Fortran: **`pgf90 -acc -ta=nvidia -Minfo=accel -o saxpy_acc saxpy.f90`**
- Compiler output:

```
pgcc -acc -Minfo=accel -ta=nvidia -o saxpy_acc saxpy.c
saxpy:
      8, Generating copyin(x[:n-1])
         Generating copy(y[:n-1])
         Generating compute capability 1.0 binary
         Generating compute capability 2.0 binary
      9, Loop is parallelizable
         Accelerator kernel generated
          9, #pragma acc loop worker, vector(256) /* blockIdx.x threadIdx.x */
             CC 1.0 : 4 registers; 52 shared, 4 constant, 0 local memory bytes; 100% occupancy
             CC 2.0 : 8 registers; 4 shared, 64 constant, 0 local memory bytes; 100% occupancy
```

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: $\nabla^2 f(x, y) = 0$



$$A_{k+1}(i,j) = \frac{A_k(i-1,j) + A_k(i+1,j) + A_k(i,j-1) + A_k(i,j+1)}{4}$$

JACOBI ITERATION C CODE

```
while ( error > tol && iter < iter_max ) {
  error=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]);


      error = max(error, 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

JACOBI ITERATION FORTRAN CODE

```
do while ( err > tol .and. iter < iter_max )
  err=0._fp_kind
  do j=1,m
    do i=1,n
      Anew(i,j) = .25_fp_kind * (A(i+1, j  ) + A(i-1, j  ) + &
                                 A(i  , j-1) + A(i  , j+1))
      err = max(err, Anew(i,j) - A(i,j))
    end do
  end do
  do j=1,m-2
    do i=1,n-2
      A(i,j) = Anew(i,j)
    end do
  end do
  iter = iter +1
end do
```

Iterate until converged

Iterate across matrix elements

Calculate new value from neighbors

Compute max error for convergence

Swap input/output arrays

EXERCISES

General instructions (compiling)

- Exercises are in “exercises/openacc” directory
  - Solutions in “exercise_solutions/openacc” directory
- To compile, use one of the provided makefiles
  - C: `> make`
  - Fortran: `> make -f Makefile_f90`
- Remember these flags
  - `-acc -ta=nvidia -Minfo=accel`

EXERCISES

General instructions (running)

To run, use `sbatch` with one of the provided job files

```
> sbatch runit.acc
> qstat -u <username>          # prints qsub status
```

Output is placed in `slurm.*` when finished.

EXERCISE 1

Jacobi kernels

- Task: use `acc kernels` to parallelize the Jacobi loop nests
- Edit laplace2D.c or laplace2D.f90 (your choice)
  - In the `001-laplace2D-kernels` directory
  - Add directives where it helps
  - Figure out the proper compilation flags to use
  - Optionally: Run OpenMP version with `laplace_omp`
- Q: can you get a speedup with just kernels directives?
  - Versus 1 CPU core? Versus 6 CPU cores?

EXERCISE 1 SOLUTION: OPENACC C

```
while ( error > tol && iter < iter_max ) {
  error=0.0;

#pragma acc kernels
  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]);

      error = max(error, abs(Anew[j][i] - A[j][i]);
    }
  }

#pragma acc kernels
  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }

  iter++;
}
```

Execute GPU kernel for loop nest

Execute GPU kernel for loop nest

EXERCISE 1 SOLUTION: OPENACC FORTRAN

```
do while ( error > tol .and. iter < iter_max )
  err=0._fp_kind

$!acc kernels
  do j=1,m
    do i=1,n

      Anew(i,j) = 0.25 * (A(i+1,j) + A(i-1,j) + &
                          A(i,j-1) + A(i,j+1))

      err = max(err, abs(Anew(i,j) - A(i,j);
    enddo
  enddo
!$acc end kernels

!$acc kernels
  do j=1, m-2
    do i=1,n-2
      A(i,j) = Anew(i,j)
    enddo
  enddo
!$acc end kernels
  iter = iter+1
enddo
```

Execute GPU kernel for loop nest

Execute GPU kernel for loop nest

EXERCISE 1: COMPILER OUTPUT (C)

```
pgcc -tp sandybridge-64 -acc -ta=nvidia -Minfo=accel -o laplace2d_acc laplace2d.c
main:
     56, Generating present_or_copyout(Anew[1:4094][1:4094])
         Generating present_or_copyin(A[:][:])
         Generating Tesla code
     57, Loop is parallelizable
     59, Loop is parallelizable
         Accelerator kernel generated
         57, #pragma acc loop gang /* blockIdx.y */
         59, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
         63, Max reduction generated for error
     68, Generating present_or_copyin(Anew[1:4094][1:4094])
         Generating present_or_copyout(A[1:4094][1:4094])
         Generating Tesla code
     69, Loop is parallelizable
     71, Loop is parallelizable
         Accelerator kernel generated
         69, #pragma acc loop gang /* blockIdx.y */
         71, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
```

EXERCISE 1: PERFORMANCE

CPU: Intel E5-2670
8 Cores @ 2.60 GHz

GPU: NVIDIA Tesla K520m

Execution (4096x4096)	Time (s)	Speedup
CPU 1 OpenMP thread	81.2	--
CPU 2 OpenMP threads	42.4	1.91x
CPU 4 OpenMP threads	25.7	3.16x
CPU 8 OpenMP threads	21.6	5.35x
OpenACC GPU	148.5	0.15x FAIL

Speedup vs. 1 CPU core

Speedup vs. 8 CPU cores

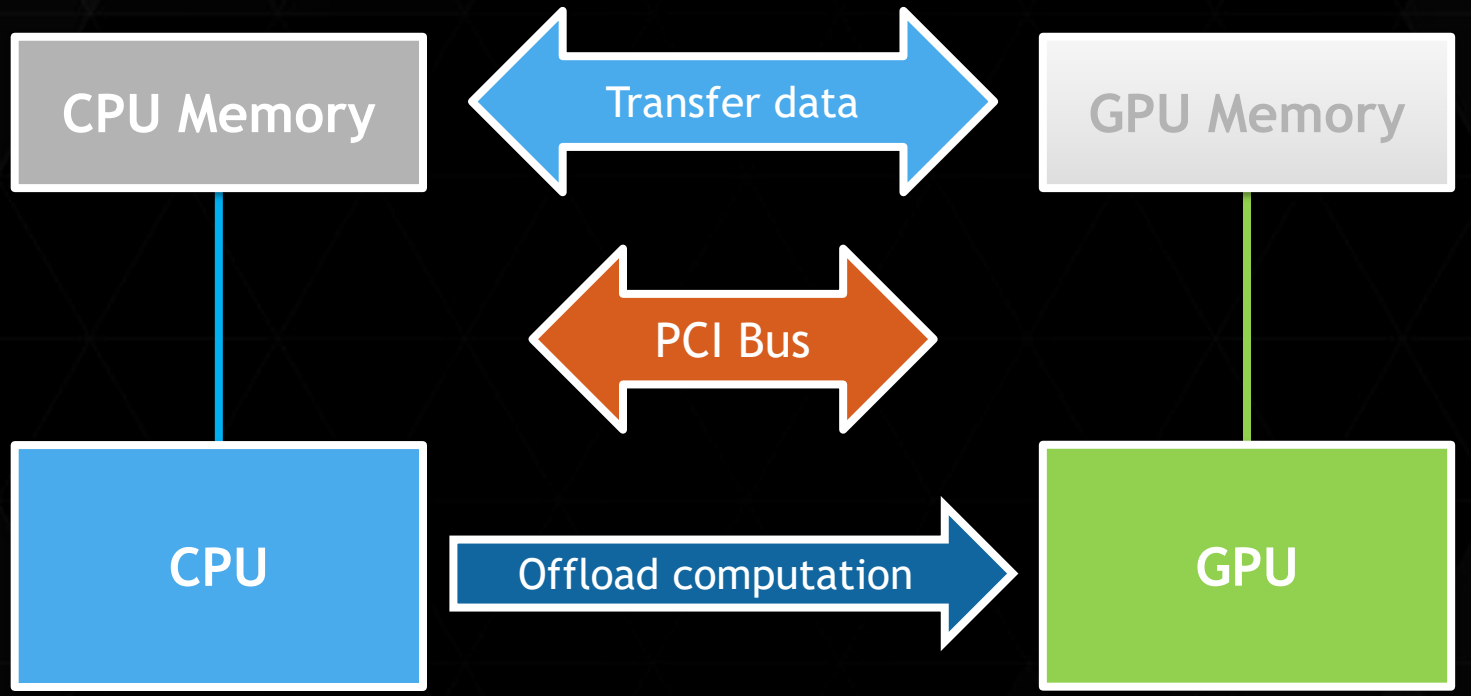
WHAT WENT WRONG?

PGI_ACC_TIME=1

```
time(us): 8,287,436
  56: data region reached 1000 times
      56: data copyin transfers: 8000
           device time(us): total=182,302 max=52 min=7 avg=22
      68: data copyout transfers: 8000
           device time(us): total=226,025 max=118 min=7 avg=28
  56: compute region reached 1000 times
      59: kernel launched 1000 times
          grid: [32x4094]  block: [128]
           device time(us): total=5,000,928 max=5,004 min=4,999 avg=5,000
          elapsed time(us): total=5,045,006 max=6,686 min=5,038 avg=5,045
      59: reduction kernel launched 1000 times
          grid: [1]  block: [256]
           device time(us): total=239,763 max=241 min=239 avg=239
          elapsed time(us): total=262,790 max=332 min=259 avg=262
  68: data region reached 1000 times
      68: data copyin transfers: 8000
           device time(us): total=232,372 max=106 min=26 avg=29
      77: data copyout transfers: 8000
           device time(us): total=225,290 max=320 min=7 avg=27
  68: compute region reached 1000 times
      71: kernel launched 1000 times
          grid: [32x4094]  block: [128]
           device time(us): total=2,182,750 max=2,186 min=2,178 avg=2,182
          elapsed time(us): total=2,226,348 max=2,458 min=2,220 avg=2,226
```

Huge Data Transfer Bottleneck!
Computation: 10 seconds
Data malloc/movement: 138

BASIC CONCEPTS



For efficiency, decouple data movement and compute off-load

EXCESSIVE DATA TRANSFERS

```
while ( error > tol && iter < iter_max ) {
  error=0.0;
```

A, Anew resident on host

Copy

```
#pragma acc kernels
```

A, Anew resident on accelerator

```
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]);
    error = max(error, abs(Anew[j][i] - A[j][i]);
  }
}
```

These copies happen every iteration of the outer while loop!*

A, Anew resident on accelerator

Copy

A, Anew resident on host

```
  ...
}
```

*Note: there are two #pragma acc kernels, so there are 4 copies per while loop iteration!

Data Management

DATA CONSTRUCT

Fortran

```
!$acc data [clause …]
    structured block
!$acc end data
```

C

```
#pragma acc data [clause …]
    { structured block }
```

General Clauses

```
if( condition )

async( expression )
```

Manage data movement. Data regions may be nested.

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.
`copyin ( list )`	Allocates memory on GPU and copies data from host to GPU when entering region.
`copyout ( list )`	Allocates memory on GPU and copies data to the host when exiting region.
`create ( list )`	Allocates memory on GPU but does not copy.
`present ( list )`	Data is already present on GPU from another containing data region.

and `present_or_copy[in|out]`, `present_or_create`, `deviceptr`.

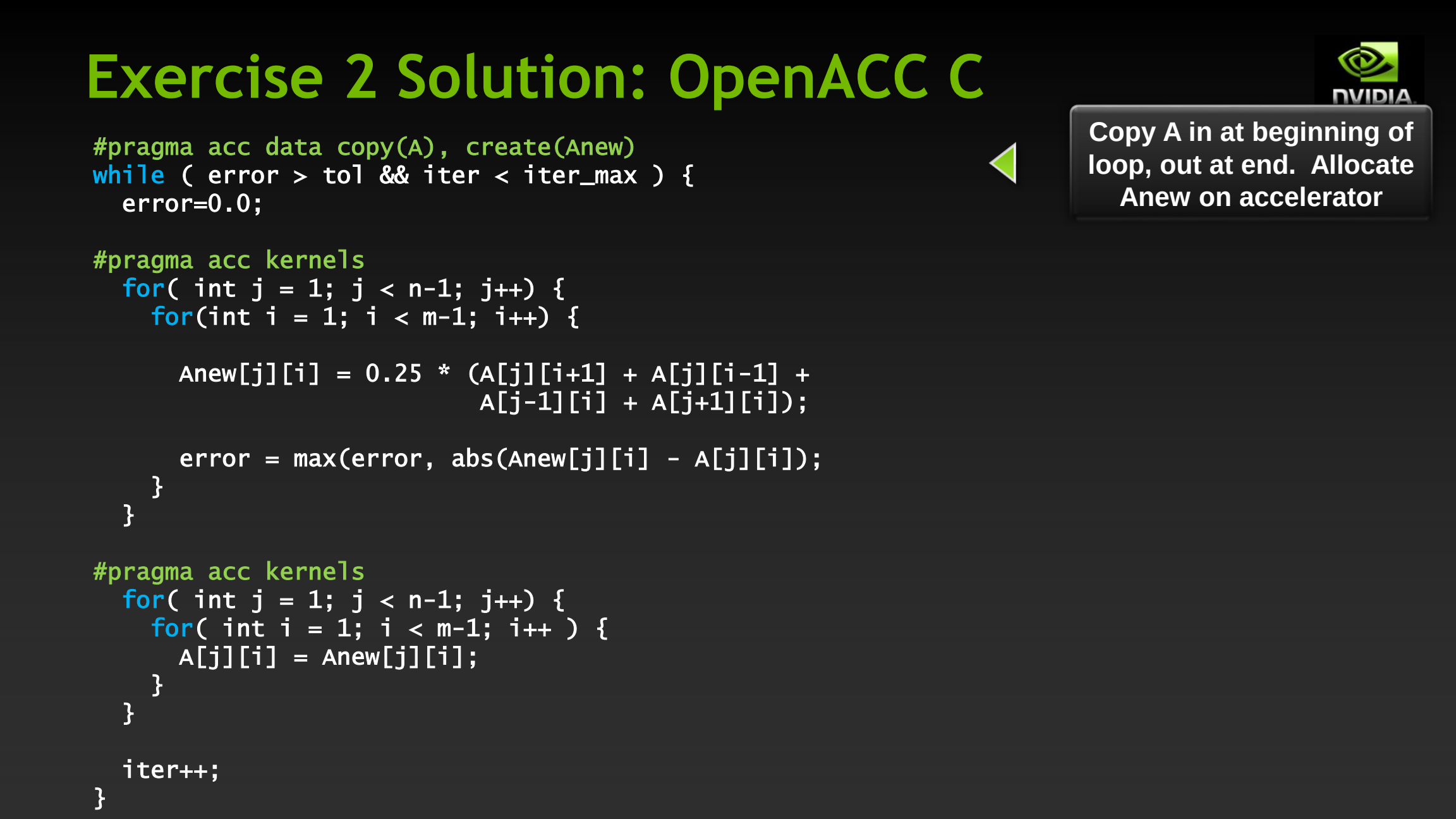
ARRAY SHAPING

- Compiler sometimes cannot determine size of arrays
  - Must specify explicitly using data clauses and array “shape”
- C
  - `#pragma acc data copyin(a[0:size-1]), copyout(b[s/4:3*s/4])`
- Fortran
  - `!$pragma acc data copyin(a(1:size)), copyout(b(s/4:3*s/4))`
- Note: data clauses can be used on `data`, `kernels` or `parallel`

EXERCISE 2: JACOBI DATA DIRECTIVES

- Task: use `acc data` to minimize transfers in the Jacobi example
- Start from given laplace2D.c or laplace2D.f90 (your choice)
  - In the `002-laplace2d-data` directory
  - Add directives where it helps (hint: [do] while loop)
- Q: What speedup can you get with data + kernels directives?
  - Versus 6 CPU cores?
  - `OMP_NUM_THREADS=6 ./laplace2d_omp`

Exercise 2 Solution: OpenACC C



```
#pragma acc data copy(A), create(Anew)
while ( error > tol && iter < iter_max ) {
  error=0.0;

#pragma acc kernels
  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]);

      error = max(error, abs(Anew[j][i] - A[j][i]);
    }
  }

#pragma acc kernels
  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 in at beginning of loop, out at end. Allocate Anew on accelerator

Exercise 2 Solution: OpenACC Fortran


```
!$acc data copy(A), create(Anew)
do while ( err > tol .and. iter < iter_max )
  err=0._fp_kind

!$acc kernels
  do j=1,m
    do i=1,n

      Anew(i,j) = .25_fp_kind * (A(i+1, j  ) + A(i-1, j  ) + &
                                 A(i  , j-1) + A(i  , j+1))

      err = max(err, Anew(i,j) - A(i,j))
    end do
  end do
!$acc end kernels

  ...

iter = iter +1
end do
!$acc end data
```

Copy A in at beginning of loop, out at end. Allocate Anew on accelerator

EXERCISE 2: PERFORMANCE

Execution (4096x4096)	Time (s)	Speedup
CPU 8 OpenMP thread	21.6	--
OpenACC K520m	148.5	0.15x
OpenACC K520m-opt	7.75	2.79x

Speedup vs. 8 CPU cores

WHAT WENT RIGHT?

```
time(us): 7,423,576
  50: data region reached 1 time
      50: data copyin transfers: 16
           device time(us): total=305 max=35 min=8 avg=19
      82: data copyout transfers: 18
           device time(us): total=182 max=28 min=1 avg=10
  56: compute region reached 1000 times
      59: kernel launched 1000 times
          grid: [32x4094]  block: [128]
           device time(us): total=5,000,403 max=5,003 min=4,998 avg=5,000
          elapsed time(us): total=5,026,969 max=5,194 min=5,020 avg=5,026
      59: reduction kernel launched 1000 times
          grid: [1]  block: [256]
           device time(us): total=239,865 max=242 min=239 avg=239
          elapsed time(us): total=261,417 max=502 min=258 avg=261
  68: compute region reached 1000 times
      71: kernel launched 1000 times
          grid: [32x4094]  block: [128]
           device time(us): total=2,182,821 max=2,187 min=2,179 avg=2
          elapsed time(us): total=2,205,088 max=3,778 min=2,198 avg=
```

Transfer Bottleneck Eliminated!
Computation: 10 seconds
Data movement: negligible

FURTHER SPEEDUPS

- OpenACC gives us more detailed control over parallelization
  - Via gang, worker, and vector clauses
- By understanding more about OpenACC execution model and GPU hardware organization, we can get higher speedups on this code
- By understanding bottlenecks in the code via profiling, we can reorganize the code for higher performance
- Will tackle these in later exercises

FINDING PARALLELISM IN YOUR CODE

- (Nested) for loops are best for parallelization
- Large loop counts needed to offset GPU/memcpy overhead
- Iterations of loops must be independent of each other
  - To help compiler: `restrict` keyword (C), `independent` clause
- Compiler must be able to figure out sizes of data regions
  - Can use directives to explicitly control sizes
- Pointer arithmetic should be avoided if possible
  - Use subscripted arrays, rather than pointer-indexed arrays.
- Function calls within accelerated region must be inlineable.

TIPS AND TRICKS

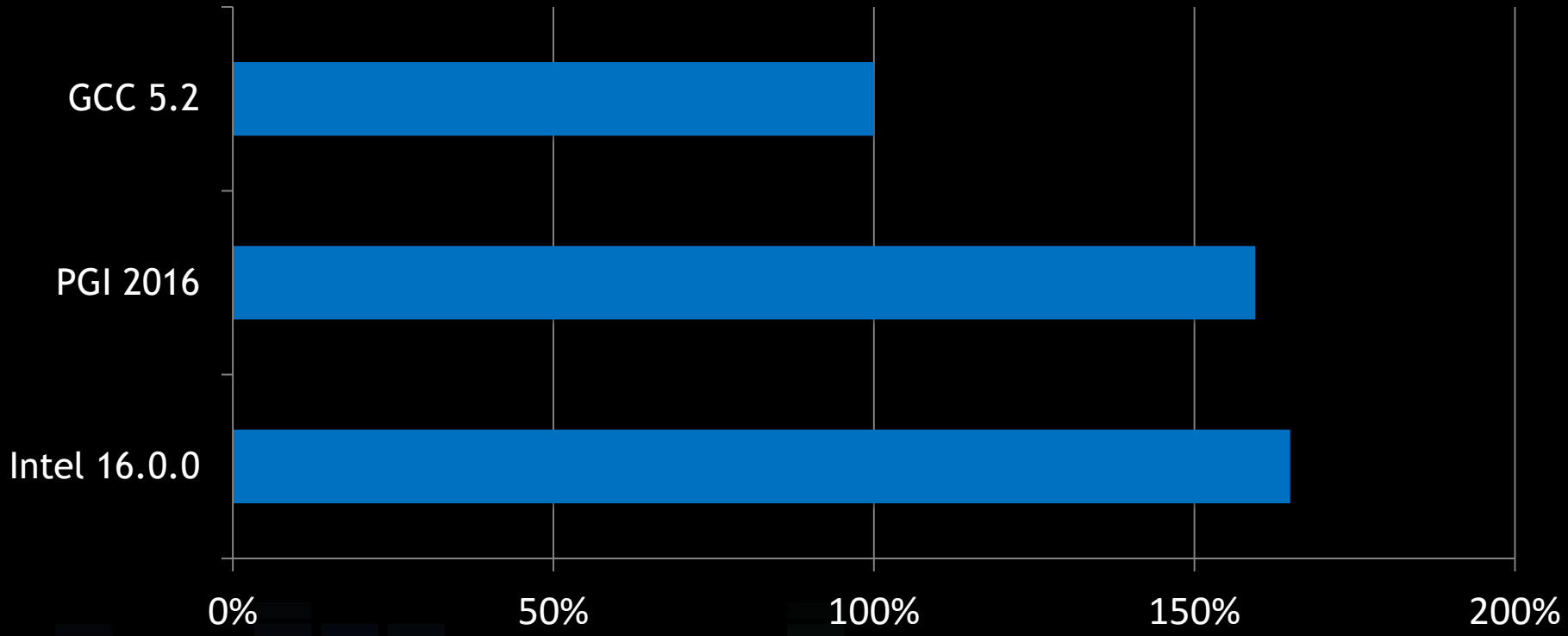
- (PGI) Use time option to learn where time is being spent
  - -ta=nvidia,time
- Eliminate pointer arithmetic
- Inline function calls in directives regions
  - (PGI): -inline or –inline,levels(<N>)
- Use contiguous memory for multi-dimensional arrays
- Use data regions to avoid excessive memory transfers
- Conditional compilation with _OPENACC macro

PGI 2016 Key New Features

- CPU
  - C++14, C++ performance optimizations
  - OpenMP and Haswell performance optimizations
  - OpenPOWER Alpha release update
- GPU
  - App's-driven features and fixes
  - OpenACC 2.5 features
  - Performance improvements
- Tools
  - All-new CPU+GPU performance profiler

PGI®

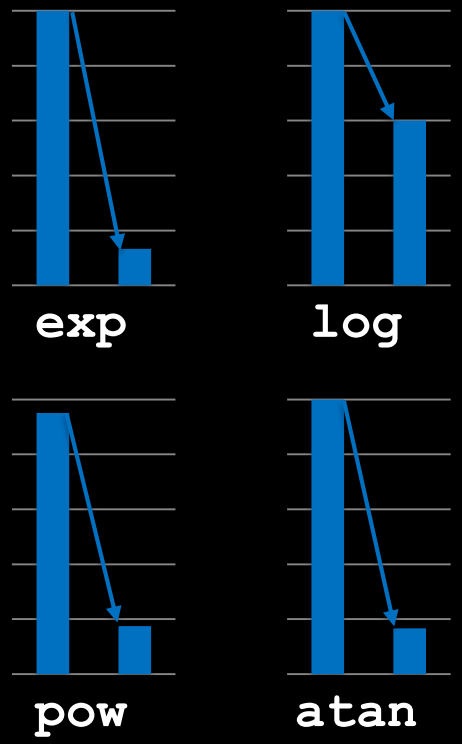
PGI 2016: World-class OpenMP for Haswell



System: 2 x Intel(R) Xeon(R) CPU E5-2698 v3 @ 2.30GHz (32 cores, 64 threads total) 128GB memory
SPECompG_base2012 relative performance as measured by PGI during the weeks of Feb. 1 and Feb. 15, 2016.
SPEComp® is a registered trademark of the Standard Performance Evaluation Corporation (SPEC).

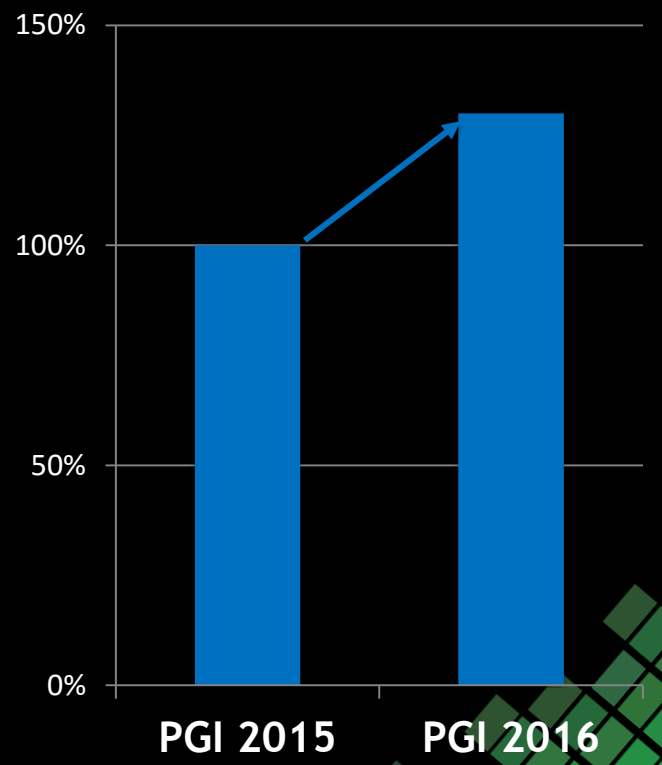
PGI 2016: Fortran Performance Improvements

Cycles per element



Faster Numerical Intrinsics + More SIMD Vectorization

25% Faster WRF Performance



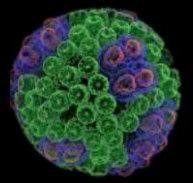
PGI®

PGI 2016: OpenACC Compilers

Environment

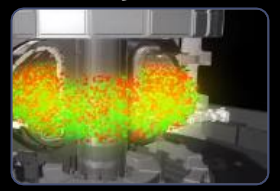
COSMO · NIM · ACME
SAMI – FV3 - COAMPS

Chemistry



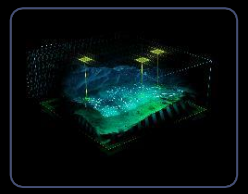
GAUSSIAN · LS-Dalton
VWM · NekCEM

Physics

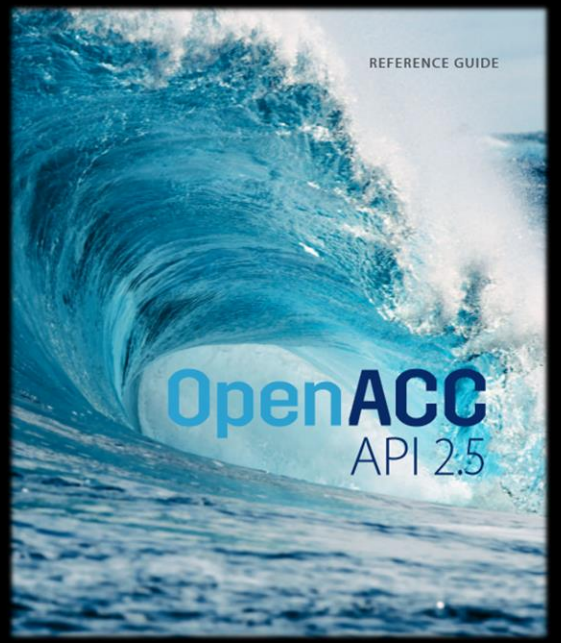


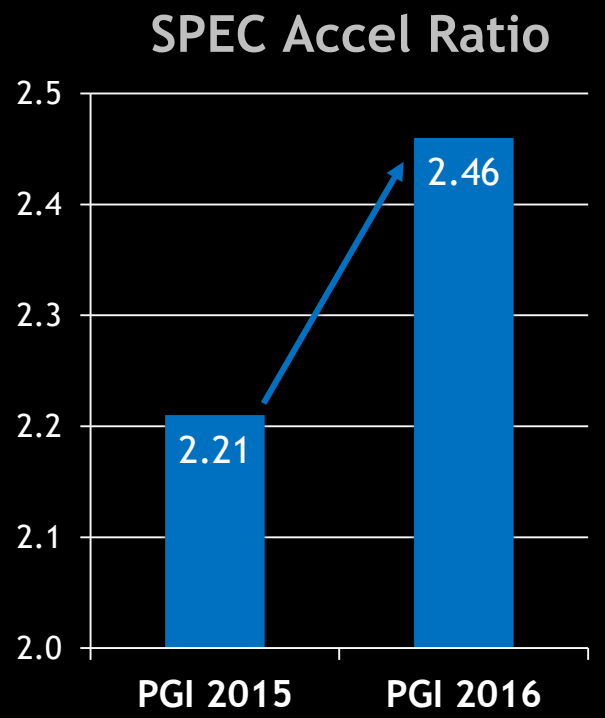
CloverLeaf – GENE

CFD



Fun3D · Fluent· HiPSTAR
INCOMP3D · NUMECA





Applications-driven Features and Tuning

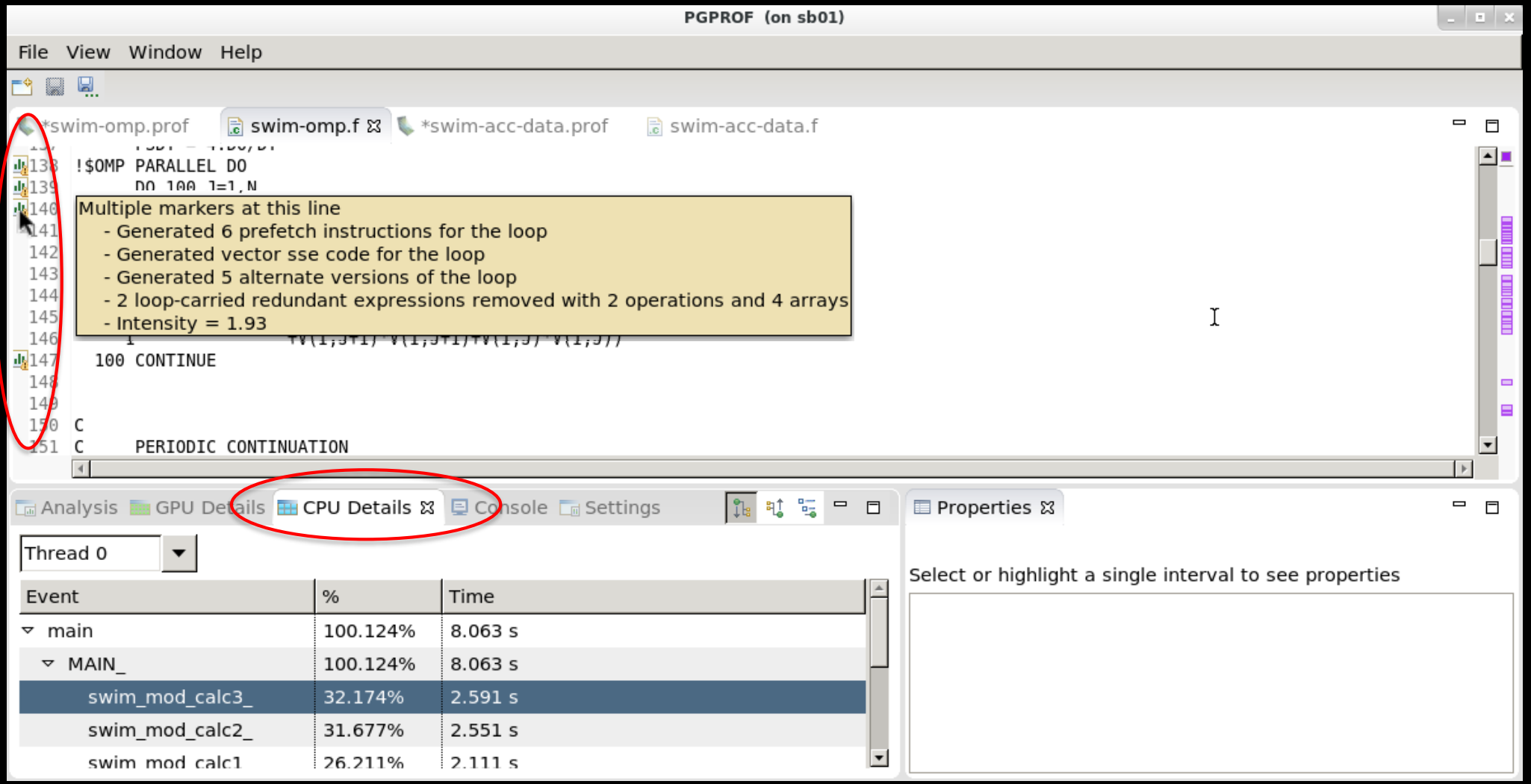
OpenACC 2.5 Features

11% Faster!

PGI®

System: Intel(R) Core™ i7 3930K CPU @ 3.2 GHz (6 cores total) 16GB memory with NVIDIA Tesla K40c GPU @ 745 MHz. SPECaccel_acc_base relative performance as measured by PGI during the weeks of Feb. 15, 2016. SPECaccel™ is a trademark of the Standard Performance Evaluation Corporation (SPEC).

PGPROF 2016: CPU Profiling, Compiler Feedback



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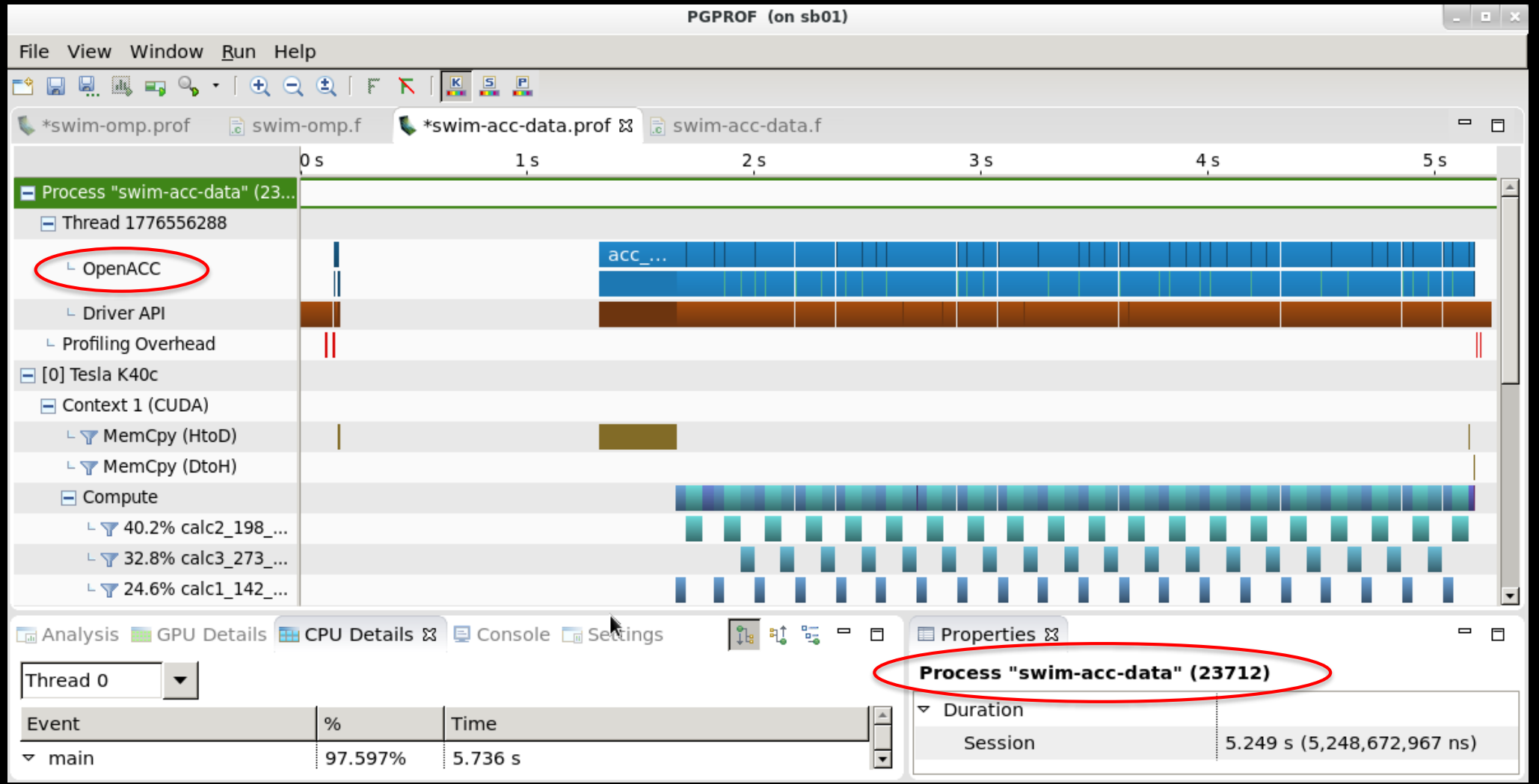
PGPROF 2016: OpenACC Profiling



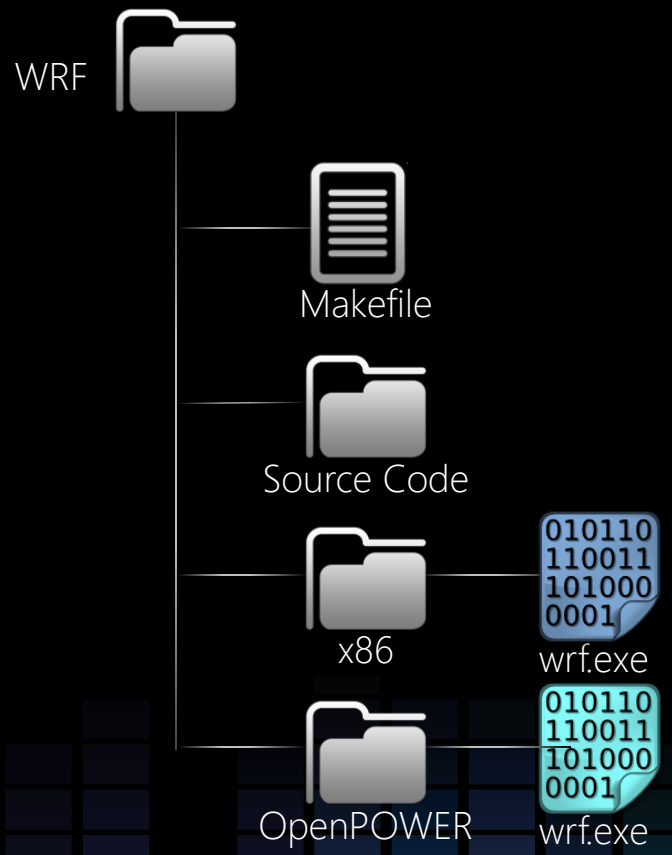
PGI®

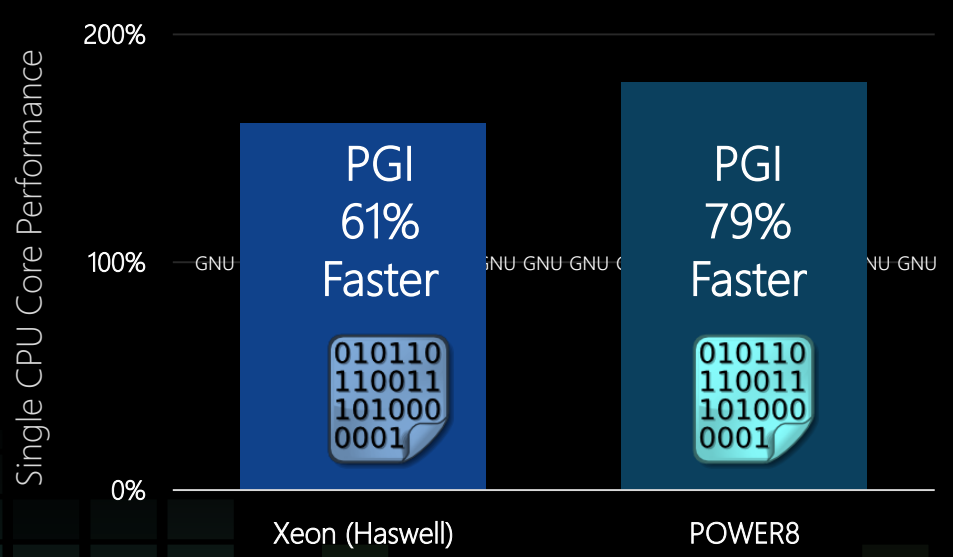
PGI 16.1-alpha for OpenPOWER+Tesla

- Feature parity with PGI Compilers on Linux/x86+Tesla
- CUDA Fortran, OpenACC, OpenMP, CUDA C/C++ host compiler
- Integrated with IBM's optimized LLVM / OpenPower code generator
- Beta release early in 2016, production later in 2016

Porting WRF from x86 to OpenPOWER

Recompile, Run





X86 CPU: Intel Xeon E5-2698 v3, 2 sockets, 32 cores total
POWER CPU: IBM 8247-42L POWER8E, 20 physical cores total
GNU version 5.2.0; PGI version 15.10

2016 OpenACC Toolkit

PGI Compiler
Free OpenACC compiler for academia

PGPROF Profiler
Easily find where to add compiler directives

Code Samples
Learn from examples of real-world algorithms

Documentation
Quick start guide, Best practices, Forums

PGI®

Download at http://developer.nvidia.com/openacc