MHPC 2023

OpenACC: Directive-based Programming For Hardware Accelerators

Programming Hardware Accelerators

Scientific Applications

Software Libraries

Drop-in Replacement of Relevant Functions

- Easy of use
- Performance guarantee
- Fixed interface

Compiler directives

Easy Acceleration of Custom Code

- Portable
- Full assistance of the compiler

Programming Languages

- Flexibility of implementation
- Steep learning curve
- Maximum performance
- Error Prone

Not for beginners

OpenACC in a Nutshell

- Directives in
 - pragmas (C, C++) or
 - comments Fortran
- Multiple parallelism levels
- Portable across
 - Accelerators
 - NVIDIA GPUs
 - Sunway
 - PEZY-SC
 - Including CPU target
 - Compilers
 - GNU GCC 9 (OpenACC 2.6)
 - PGI, ...
- Performance
 - Often close to "native" efficiency

```
int main(void) {
    // host code
    #pragma acc kernels
    {
        // accelerated code
    }
    return 0;
}
```

OpenACC Main Features

Incremental

- Sequential code preserved
- Annotations limited to important parts of the code
 - Profile-based performance tuning
- Correctness verified as needed without massive code changes

Single Source

- Same code for sequential and accelerated code
- Recompile on a new platform for performance
- Sequential code unaffected and developed in unison

Ease of use

- Gentle learning curve
- Works for HPC languages: C, C++, Fortran
- No low-level hardware experience or details required

Jacobi Iteration: C Code

```
Iterate until convergence
while ( err > tol && iter < iter max ) {</pre>
   err=0.0;
                                                              Iterate across matrix elems.
   for ( int j = 1; j < n-1; j++) {
       for (int i = 1; i < m-1; i++) {
                                                                 Calculate new value
          Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                                                                   from neighbors
                                  A[j-1][i] + A[j+1][i]);
                                                                 Compute max-error
          err = max(err, abs(Anew[j][i] - A[j][i]));
                                                                  for convergence
   for ( int j = 1; j < n-1; j++) {
                                                               Swap input/output arrays
       for ( int i = 1; i < m-1; i++ ) {
          A[j][i] = Anew[j][i];
```

iter++;

OpenACC Syntax Overview

- A pragma in C and C++
 - Instructs the compiler how to compile the code
 - Compilers may ignore pragma they don't understand
- Specially formatted comment is required in Fortran
 - Comments can be ignored by the compiler
- acc starts OpenACC directives and clauses
- Directives are commands for OpenACC compiler to alter the following code
- Clauses are augment directives with extra details and functionality

OpenACC Directives

```
Manage
Data
              #pragma acc data copyin(x,y) copyout(z)
Movement
                 /* ... */
Initiate
                 #pragma acc parallel
Parallel
Execution_
  Optimize
                 #pragma acc loop gang vector
   Loop
                     for (i = 0; i < n; ++i) {
  Mappings
                          z[i] = x[i] + y[i];
                          /* ... */
                                             OpenACC
                                       Directives for Accelerators
```

- Incremental
- Single source
- Interoperable
- Performance portable
- CPU, GPU, Xeon Phi

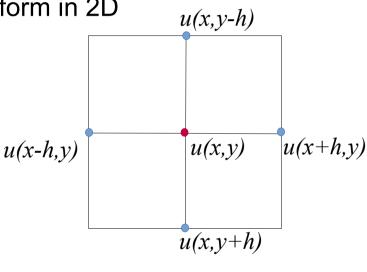
OpenACC Example: Stencil Code with DATA and KERNELS

```
#pragma acc data copy(b[0:n][0:m]) create(a[0:n][0:m])
for (iter = 1; iter <= p; ++iter) {</pre>
   #pragma acc kernels
   for (i = 1; i < n-1; ++i) {
      for (j = 1; j < m-1; ++j) {
          a[i][j]=w0*b[i][j]+
                  w1*(b[i-1][j]+b[i+1][j]+
                       b[i][j-1]+b[i][j+1])+
                   w2*(b[i-1][j-1]+b[i-1][j+1]+
                       b[i+1][j-1]+b[i+1][j+1]);
   for (i = 1; i < n-1; ++i)
      for( j = 1; j < m-1; ++j )
b[i][j] = a[i][j];</pre>
```

Example: Jacobi Iteration for Poisson Equation

- Poisson equation has a simple form in 2D
- $u_{xx} + u_{yy} = f(x,y)$
- Applications include
 - Electricity
 - Magnetism
 - Gravity
 - Heat distribution
 - Fluid flow
 - Fluid How
 - Torsion $\nabla^2 f(x, y) = 0$
- When f(x,y)=0 we call it Laplace equation

$$u_{xx} = \frac{\partial^2 u}{\partial x \partial x} \approx \frac{u(x+h,y) - 2u(x,y) + u(x-h,y)}{h^2}$$
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Jacobi Iteration: C Code

```
Iterate until convergence
while ( err > tol && iter < iter max ) {</pre>
   err=0.0;
                                                              Iterate across matrix elems.
   for ( int j = 1; j < n-1; j++) {
       for (int i = 1; i < m-1; i++) {
                                                                 Calculate new value
          Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                                                                   from neighbors
                                   A[j-1][i] + A[j+1][i]);
                                                                  Compute max-error
          err = max(err, abs(Anew[j][i] - A[j][i]));
                                                                   for convergence
   for ( int j = 1; j < n-1; j++) {
                                                               Swap input/output arrays
       for ( int i = 1; i < m-1; i++ ) {
```

A[j][i] = Anew[j][i];

iter++;

Looking for Parallelism

```
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]));
```

Max reduction required

Data dependence

between iterations

Independent loop iterations

for (int j = 1; j < n-1; j++) { for (int i = 1; i < m-1; i++) { A[j][i] = Anew[j][i];

iter++;

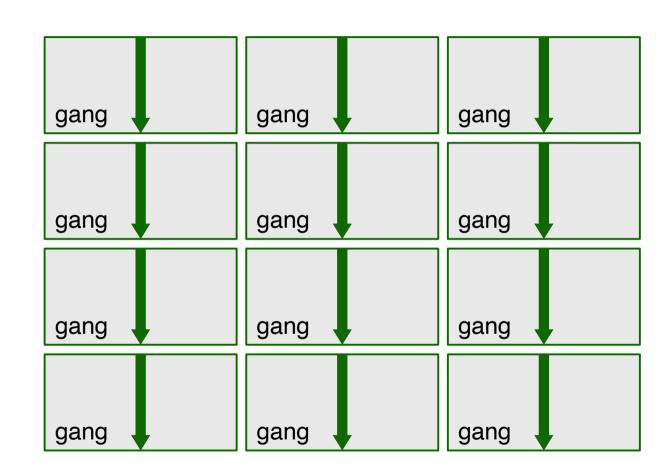
Independent loop iterations

OpenACC Parallel Directive

Generates parallelism

```
#pragma acc parallel
{
```

When encountering the parallel directive, the compiler will generate 1 or more parallel gangs, which execute redundantly.

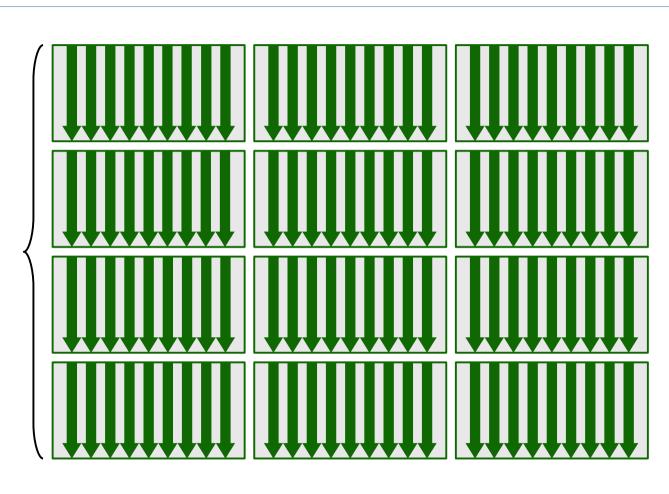


OpenACC Loop Directive

Identifies loops to run in parallel

```
#pragma acc parallel
{
    #pragma acc loop
    for (i=0; i<N; ++i)
    {
     }
}</pre>
```

The loop directive informs the compiler which loops to parallelize.

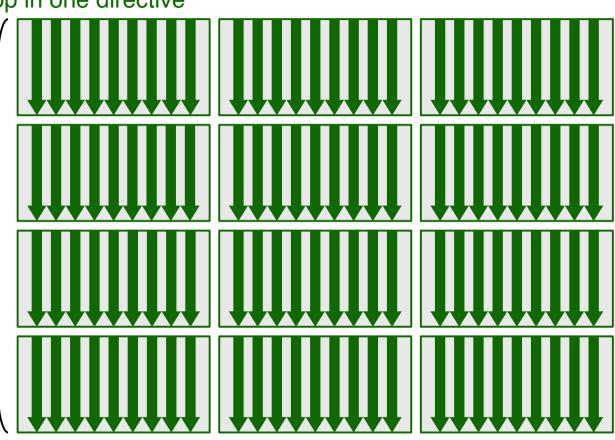


OpenACC Parallel Loop Directive

Generates parallelism and identifies loop in one directive

```
#pragma acc parallel loop
for (i=0; i<N; ++i)
{
}</pre>
```

The parallel and loop directives are frequently combined into one.



Looking for Parallelism

```
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]));
```

Parallelize loop on

accelerator

Parallelize loop on accelerator

for (int i = 1; i < m-1; i++) { A[j][i] = Anew[j][i];A reduction means that all n*m values for err will be reduced to just one, the max.

iter++;

#pragma acc parallel loop

for (int j = 1; j < n-1; j++) {

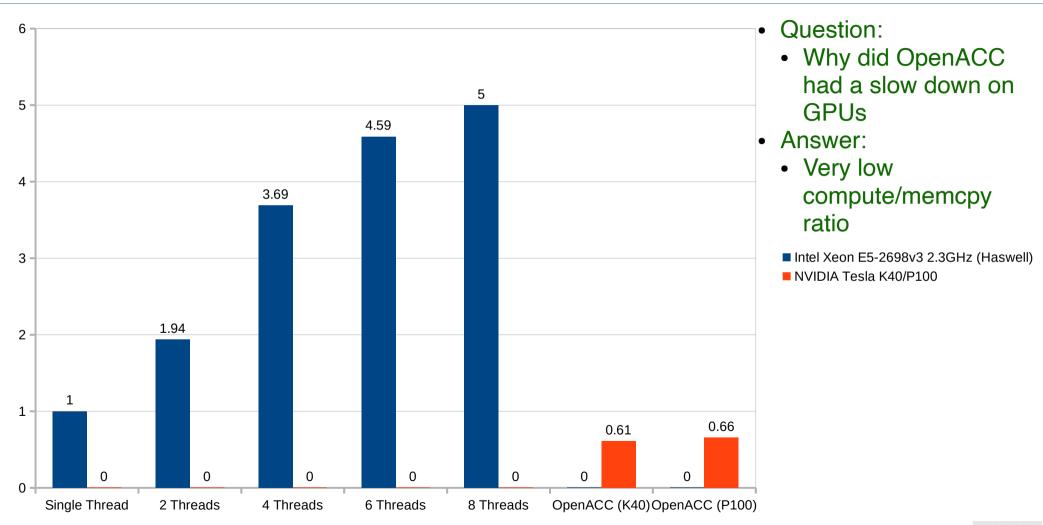
OpenACC Loop Directive: PRIVATE & REDUCTION

- The private and reduction clauses are not optimization clauses, the may be required for correctness.
- Private = a copy of the variable is made for each loop iteration
- Reduction = a reduction is performed on the listed variables
 - Supports: +, *, max, min, and logical operators

Building OpenACC Code with PGI Compiler

```
$ pgcc -fast -acc -ta=tesla -Minfo=all laplace2d.c
main:
40, Loop not fused: function call before adjacent loop
    Generated vector sse code for the loop
51, Loop not vectorized/parallelized: potential early exits
55, Accelerator kernel generated
    55, Max reduction generated for error
    56, #pragma acc loop gang /* blockIdx.x */
    58, #pragma acc loop vector(256) /* threadIdx.x */
55, Generating copyout (Anew[1:4094][1:4094])
    Generating copyin(A[:][:])
    Generating Tesla code
58, Loop is parallelizable
66, Accelerator kernel generated
    67, #pragma acc loop gang /* blockIdx.x */
    69, #pragma acc loop vector(256) /* threadIdx.x */
66, Generating copyin (Anew[1:4094][1:4094])
    Generating copyout(A[1:4094][1:4094])
    Generating Tesla code
69, Loop is parallelizable
```

Performance Results: Speedup (Higher is Better)



```
while ( err > tol && iter <
                                         A, Anew resident on accelerator
iter max ) {
    err=0.0;
                                        #pragma acc parallel loop
A, Anew resident on host
                                           for ( int j = 1; j < n-1; j++) {
                            copy
                                               for (int i = 1; i < m-1; i++)
                                                  Anew[j][i] = 0.25 * (
    These copies
                                                      A[j][i+1] + A[j][i-1] +
    happen every
                                                      A[j-1][i] + A[j+1][i]);
    iteration of the
                                                  err = max(err,
   outer while loop!
                                                 abs(Anew[j][i] - A[j][i]));
A, Anew resident on host
                            copy
                                         A, Anew resident on accelerator
```

Looking for Parallelism

```
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]));
        CC Dares.
                                                     Does CPU need data
                                                   between these loop nests?
#pragma acc parallel loop
   for ( int j = 1; j < n-1; j++) {
     for ( int i = 1; i < m-1; i++ ) {
           \.....
                                                     Does CPU need data
        A[j][i] = Anew[j][i];
                                                    between iterations of the
  iter++;
```

convergence loop?

Data Regions

The data directive defines a region of code in which GPU arrays remain on the GPU and are shared among all kernels in that region.

```
#pragma acc data
{
#pragma acc parallel loop
/* . . . */

#pragma acc parallel loop
/* . . . */
}

Data region

Arrays used within the data region will remain on the GPU until the end of the data region.
```

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.
- deviceptr(list)
 - The variable is a device pointer (e.g. CUDA) and can be used directly on the device.

Array Shaping

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

Data Regions Have Real Consequences

```
int main(int argc, char** argv) {
int main(int argc, char** argv) {
                                          float A[1000];
   float A[1000];
                                       #pragma acc data copy(A)
                              Copied
                                                                     Copied
                              To GPU
                                                                    To GPU
   #pragma acc kernels
                                          #pragma acc kernels
   for( int iter = 1; iter < 1000;</pre>
                                          for( int iter = 1; iter < 1000;
        ++iter) {
                                               ++iter) {
                                                                      Still
     A[iter] = 1.0;
                               Copied
                                             A[iter] = 1.0;
                                                                    Runs on
                               To Host
                                          1 // "kernels" end here
                                                                     Host
                               Runs
                                          A[10] = 2.0;
  A[10] = 2.0;
                                 on
                                                                     Copied
                                Host
                                                                    To Host
 printf("A[10] = %f", A[10]);
                                         printf("A[10] = %f", A[10]);
           Output: A[10] = 2.0
                                                Output: A[10] = 1.0
                                                                       24/27
```

Looking for Parallelism

```
#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 Anew as a device temporary.

Building the New OpenACC Code with PGI Compiler

```
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main:
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    Generated vector sse code for the loop
51, Generating copy(A[:][:])
    Generating create (Anew[:][:])
    Loop not vectorized/parallelized: potential early exits
56, Accelerator kernel generated
    56, Max reduction generated for error
    57, #pragma acc loop gang /* blockIdx.x */
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56, Generating Tesla code
59, Loop is parallelizable
67, Accelerator kernel generated
    68, #pragma acc loop gang /* blockIdx.x */
    70, #pragma acc loop vector(256) /* threadIdx.x */
67, Generating Tesla code
70, Loop is parallelizable
```

Performance Results: Speedup (Higher is Better)

