Accelerator programming with OpenACC

Colaboratorio Nacional de Computación Avanzada

Jorge Castro
jcastro@cenat.ac.cr

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Agenda

Introduction

What is OpenACC?

OpenACC is a parallel programming standard that describes a set of compiler directives in C, C++ and Fortran to specify regions of code offloading from a host CPU to an attached accelerator

OpenACC
Directives for Accelerators

What is an Accelerator?

Dedicated piece of hardware that performs specific functions faster than a CPU

- Graphic Processing Unit (GPU): electronic device that runs computer graphic algorithms to render images
- Coprocessor: electronic device to supplement functions of CPU (arithmetic, encryption, error detection)

Top 500 green

Rank	TOP500 Rank	System	Cores	Rmax (TFlop/s)	Power (kW)	Power Efficiency (GFlops/watts)
1	259	**Shoubu system B** - ZettaScaler-2.2, Xeon D-1571 16C 1.3GHz, Infiniband EDR, PEZY-SC2 , PEZY Computing / Exascaler Inc. Advanced Center for Computing and Communication, RIKEN Japan	794,400	842.0	50	17.009
2	307	**Suiren2** - ZettaScaler-2.2, Xeon D-1571 16C 1.3GHz, Infiniband EDR, PEZY-SC2 , PEZY Computing / Exascaler Inc. High Energy Accelerator Research Organization /KEK Japan	762,624	788.2	47	16.759
3	276	**Sakura** - ZettaScaler-2.2, Xeon E5-2618Lv3 8C 2.3GHz, Infiniband EDR, PEZY-SC2 , PEZY Computing / Exascaler Inc. PEZY Computing K.K. Japan	794,400	824.7	50	16.657
4	149	**DGX SaturnV Volta** - NVIDIA DGX-1 Volta36, Xeon E5-2698v4 20C 2.2GHz, Infiniband EDR, NVIDIA Tesla V100 , Nvidia NVIDIA Corporation United States	22,440	1,070.0	97	15.113
5	4	**Gyoukou** - ZettaScaler-2.2 HPC system, Xeon D-1571 16C 1.3GHz, Infiniband EDR, PEZY-SC2 700Mhz , ExaScaler Japan Agency for Marine-Earth Science and Technology Japan	19,860,000	19,135.8	1,350	14.173
6	13	**TSUBAME3.0** - SGI ICE XA, IP139-SXM2, Xeon E5-2680v4 14C 2.4GHz, Intel Omni-Path, NVIDIA Tesla P100 SXM2 , HPE GSIC Center, Tokyo Institute of Technology Japan	135,828	8,125.0	792	13.704

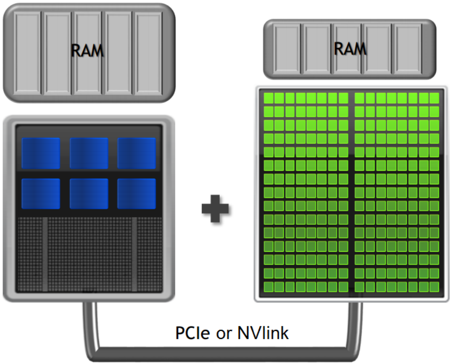
Source: www.top500.org/green500 (November 2017 list)

K40 vs P100 vs V100

Accelerator	Cores	Boost clock	Memory BW	DP perf	SP perf
Tesla k40	2880	875 MHz	288 GB/s	1.7 TFLOPS	5.0 TFLOPS
Tesla P100	3584	1480 MHz	720 GB/s	5.3 TFLOPS	10.6 TFLOPS
Tesla V100	5120	1530 MHz	900 GB/s	7.8 TFLOPS	15.7 TFLOPS

Architecture

Accelerator Nodes



CPU and GPU have distinct memories

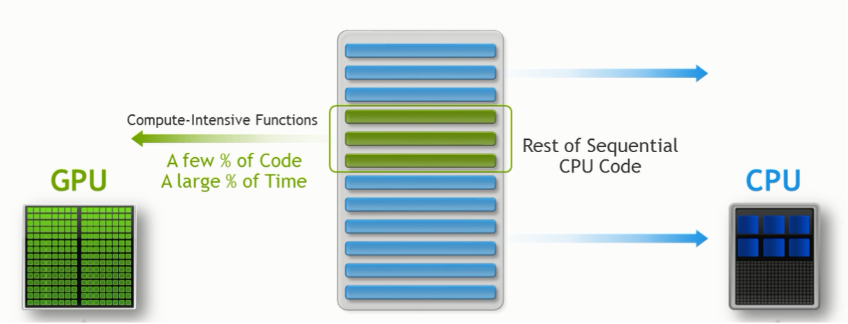
- CPU generally larger and slower
- GPU generally smaller and faster

CPU and GPU communicate via PCIe

- Data must be copied between these memories over PCIe
- PCIe Bandwidth is much lower than either memories

Heterogeneous computing

Heterogeneous programming combines the use of more than one type of processors



CPU vs GPU

Features	CPU	GPU
Main memory	large	small
Memory bandwidth	low	high
Clock Frequency	high	low
Performance per watt	low	high
Throughput[1]	low	high

[1] number of operations per unit of time

Why use OpenACC?

- Simple
- Portable (Nvidia GPUs and Intel-AMD CPUs)
- Inter-operable (CUDA, MPI, OPENMP)
- Powerful (90% CUDA)

```
main()
{
  <serial code>
  #pragma acc kernels
  //automatically runs on GPU
  {
    <parallel code>
  }
}
```

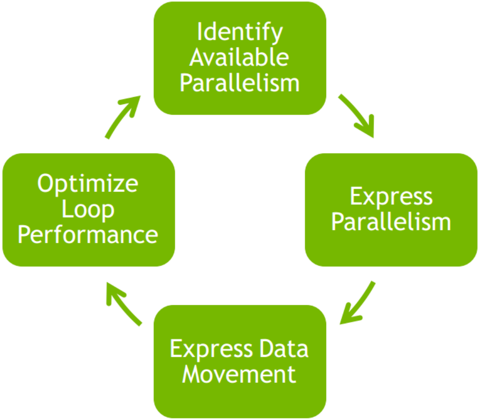
THE SUPERCOMPUTER COMPANY

Why use OpenACC? (2)

	Shared-memory Programming	Accelerator Programming	Distributed-memory Programming
High-level	OpenMP	OpenACC	Global Arrays, Charm++
Low-level	PThreads, OpenThreads	CUDA, OpenCL	MPI

OpenACC life cycle

OpenACC life cycle

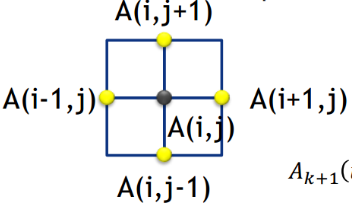


Jacobi iteration

Example: Jacobi Iteration

Stencil operation

Example: Solve Laplace equation in 2D: $\nabla^2 f(x,y) = 0$



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

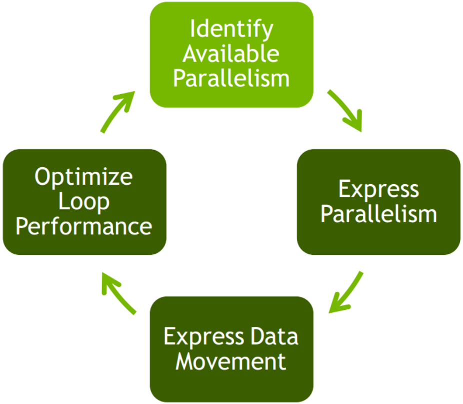
Jacobi iteration (2)

Jacobi Iteration: C Code

```
while ( err > tol && iter < iter_max ) {
  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

OpenACC life cycle



Identify parallelism

Identify Parallelism

```
while ( err > tol && iter < iter_max ) {
  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++;
}
```

Identify parallelism (2)

Identify Parallelism

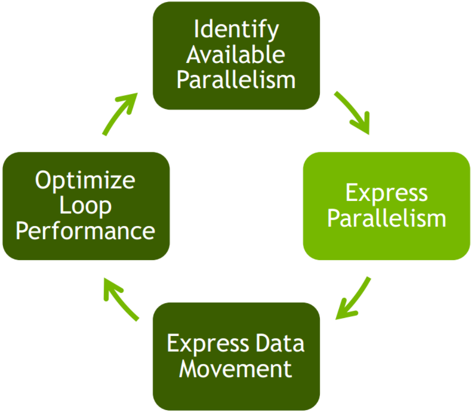
```
while ( err > tol && iter < iter_max ) {
  err=0.0;

  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++;
}
```

Data dependency between iterations.

Independent loop iterations

Independent loop iterations

OpenACC life cycle



Express parallelism

OpenACC kernels Directive

The kernels directive identifies a region that may contain *loops* that the compiler can turn into parallel *kernels*.

```
#pragma acc kernels
{
for(int i=0; i<N; i++)
{
  x[i] = 1.0;
  y[i] = 2.0;
}

for(int i=0; i<N; i++)
{
  y[i] = a*x[i] + y[i];
}
}
```

Express parallelism

OpenACC kernels Directive

The kernels directive identifies a region that may contain *loops* that the compiler can turn into parallel *kernels*.

```
#pragma acc kernels
{
for(int i=0; i<N; i++)
{
  x[i] = 1.0;
  y[i] = 2.0;
}

for(int i=0; i<N; i++)
{
  y[i] = a*x[i] + y[i];
}
}
```

kernel 1

kernel 2

The compiler identifies 2 parallel loops and generates 2 kernels.

Express parallelism (2)

OpenACC parallel loop Directive

`parallel` - Programmer identifies a block of code containing parallelism. Compiler generates a *kernel*.
`loop` - Programmer identifies a loop that can be parallelized within the kernel.

NOTE: parallel & loop are often placed together

```
#pragma acc parallel loop
for(int i=0; i<N; i++)
{
  y[i] = a*x[i]+y[i];
}
```

Generates a Parallel Kernel

Express parallelism (3)

Parallelize with OpenACC kernels

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

      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++;
}
```

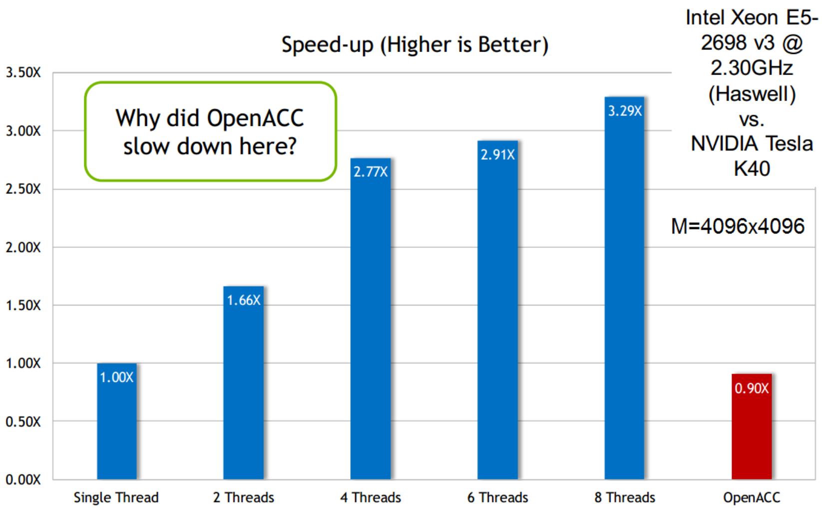
Look for parallelism within this region.

Express parallelism (4)

Building the code

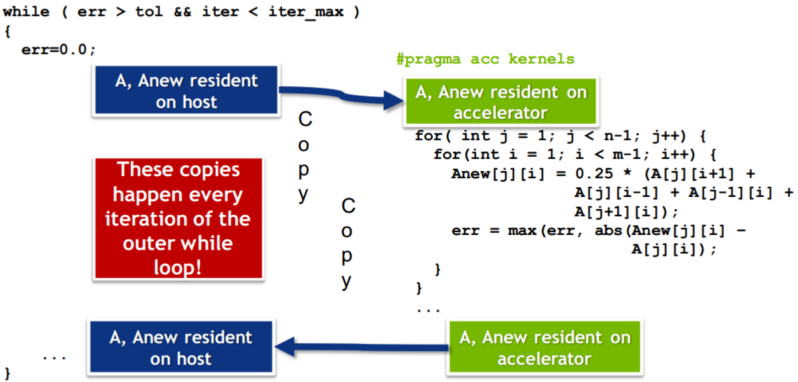
```
$ pgcc -fast -ta=tesla -Minfo=all laplace2d.c
main:
     40, Loop not fused: function call before adjacent loop
         Generated vector sse code for the loop
     51, Loop not vectorized/parallelized: potential early exits
     55, Generating copyout(Anew[1:4094][1:4094])
         Generating copyin(A[:][:])
         Generating copyout(A[1:4094][1:4094])
         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
     67, Loop is parallelizable
     69, Loop is parallelizable
         Accelerator kernel generated
         67, #pragma acc loop gang /* blockIdx.y */
         69, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
```

Express parallelism (5)



Express parallelism (6)

Excessive Data Transfers



Express parallelism (7)

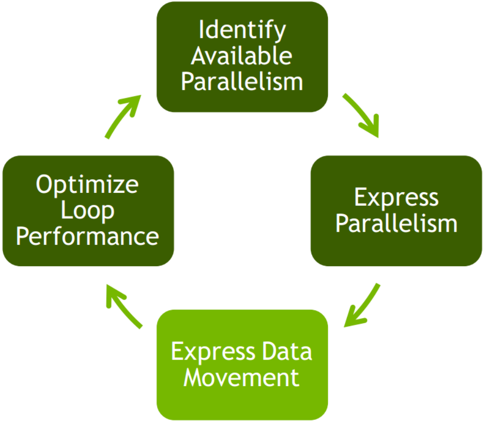
Identifying Data Locality

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

      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++;
}
```

Does the CPU need the data between these loop nests?

Does the CPU need the data between iterations of the convergence loop?

OpenACC life cycle



Express data movement

Structured 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.

Express data movement (2)

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.

Express data movement (3)

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`

Express data movement (4)

Express Data Locality

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

      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++;
}
```

Express data movement (4)

Express Data Locality

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

      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++;
}
```

Copy A to/from the accelerator only when needed.

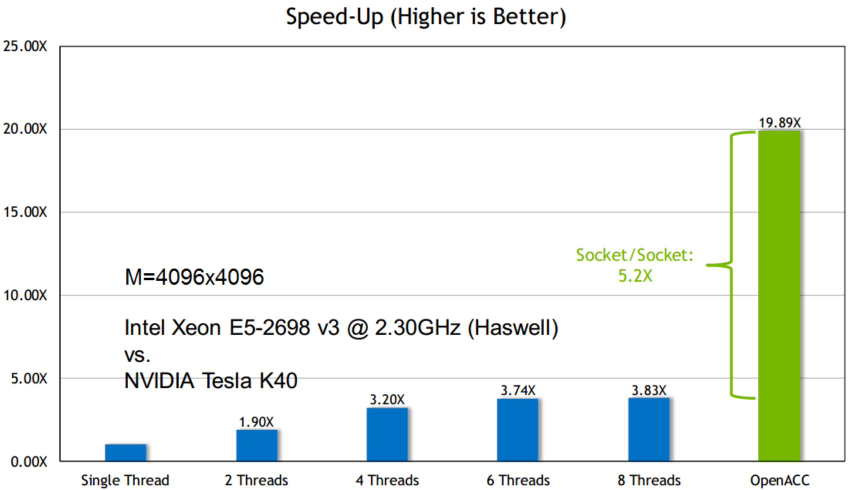
Create Anew as a device temporary.

Express data movement (5)

Rebuilding the code

```
$ 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, 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 */
         59, #pragma acc loop vector(256) /* threadIdx.x */
     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
```

Express data movement (6)



Express data movement (7)

Unstructured Data Directives

Used to define data regions when scoping doesn't allow the use of normal data regions (e.g. the constructor/destructor of a class).

`enter data` **Defines the start of an unstructured data lifetime**

- **clauses:** `copyin(list)`, `create(list)`

`exit data` **Defines the end of an unstructured data lifetime**

- **clauses:** `copyout(list)`, `delete(list)`

```
#pragma acc enter data copyin(a)
...
#pragma acc exit data delete(a)
```

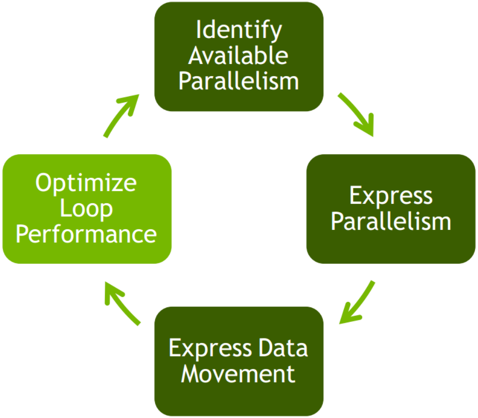
Express data movement (8)

Unstructured Data: C++ Classes

- Unstructured Data Regions enable OpenACC to be used in C++ classes
- Unstructured data regions can be used whenever data is allocated and initialized in a different scope than where it is freed (e.g. Fortran modules).

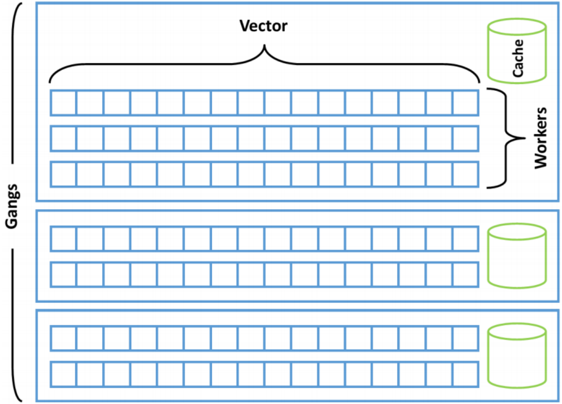
```
class Matrix {
  Matrix(int n) {
    len = n;
    v = new double[len];
#pragma acc enter data
            create(v[0:len])
  }
  ~Matrix() {
#pragma acc exit data
            delete(v[0:len])
    delete[] v;
  }

  private:
    double* v;
    int len;
};
```

OpenACC life cycle



Optimize loop performance

Levels of Parallelism



Optimize loop performance (2)

OpenACC	GPU
Vector	Thread
Worker	Warp
Gang	Thread block

Optimize loop performance (3)

The loop Directive

The `loop` directive gives the compiler additional information about the *next* loop in the source code through several clauses.

- `independent` - all iterations of the loop are independent
- `collapse(N)` - turn the next N loops into one, flattened loop
- `tile(N[,M,…])` - break the next 1 or more loops into *tiles* based on the provided dimensions.

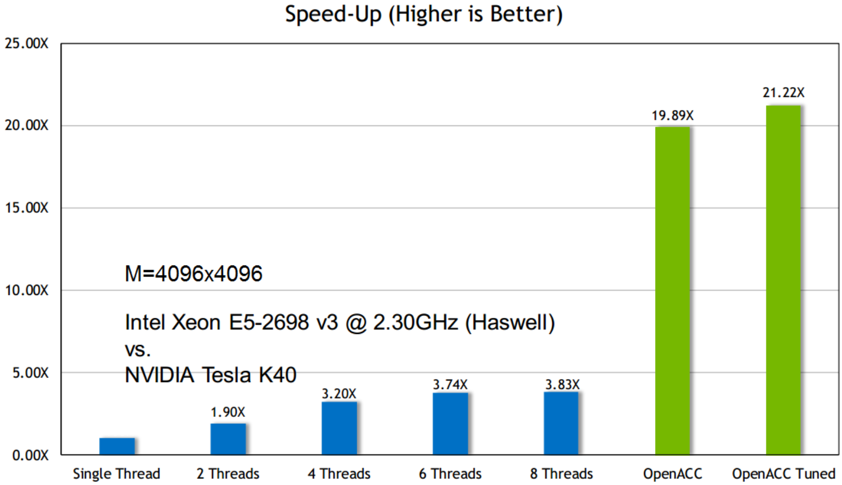
Optimize loop performance (4)

Optimize Loop Performance

```
#pragma acc data copy(A) create(Anew)
while ( err > tol && iter < iter_max ) {
  err=0.0;
#pragma acc kernels
{
#pragma acc loop device_type(nvidia) tile(32,4)
  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 loop device_type(nvidia) tile(32,4)
  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }
}
  iter++;
}
```

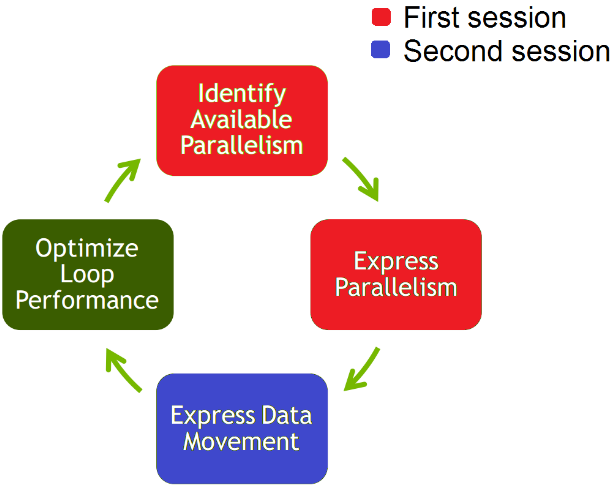
"Tile" the next two loops into 32x4 blocks, but only on NVIDIA GPUs.

Optimize loop performance (5)



Hands on session

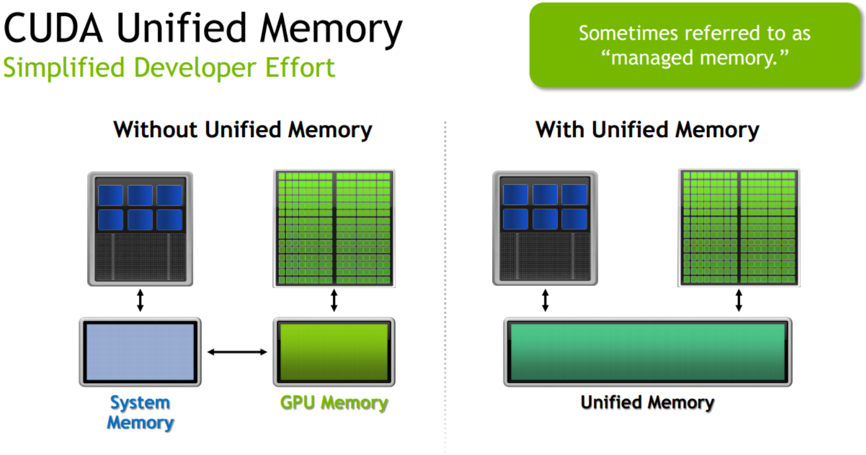
OpenACC life cycle



Profiling tools

- A profiler allows to analyze the behaviour of a program
  - Duration of function calls
  - Performance Optimization
- Graphic profiling tools
  - Nvvp, pgprof, vampir, etc
- Command-line profiling tools
  - **nvprof**, gprof, etc

CUDA Unified Memory



Nvidia OpenACC course repository

- Log into cluster Kabré
- Pull repository CRHPCS-2018

```
cd CRHPCS-2018
git pull
```

- Load CUDA toolkit

```
module load cuda/9.0.176
```

- Load pgi compiler

```
module load pgi
```

Profiling and parallelizing

- Access laboratory #2

```
cd openacc/lab2/c99/
```

- Open README file in browser

```
https://github.com/CNCA-CeNAT/CRHPCS-2018/blob/master/openacc/lab2/README.md
```

- Complete steps 0-3 (Send jobs to queue: k40)

Action	Command
Queue system	-qsub [jobName.pbs]
Check job status	watch -n 5 qstat -u USERNAME
Check GPU info	nvidia-smi

Compiler flags

- PGI C compiler: pgcc
- PGI C++ compiler: pgc++

Flag	Action
-acc	Enable OpenACC directives
-fast	Choose optimal flags for target platform
-ta=[**tesla:managed**,multicore,etc]	Specify accelerator type
-Minfo=[**accel**,all,etc]	Show compilation information

Optimizing data movement

- Access laboratory #3

```
cd openacc/lab3/c99/
```

- Open README file in browser

```
https://github.com/CNCA-CeNAT/CRHPCS-2018/blob/master/openacc/lab3/README.md
```

- Complete steps 0,1,2 and 4 (Send jobs to queue: k40)

Best practices

Optimization tips

- Use restrict keyword to avoid false loop dependencies (pointer aliasing)
- **collapse(N)**, useful when:
  - Many nested loops
  - Very small loops
- **tile(N[,M,. . .])**, useful when
  - high data locality
- Efficient **loop ordering**
  - Innermost loop iterates on fastest varying array dimension
  - Improve cache efficiency (access consecutive memory addresses)
- On **NVIDIA** devices:
  - vector lengths must be multiples of 32 (up to 1024)
  - (workers X vector) must be less than 1024

Current limitations

- **Shallow copy vs Deep copy**

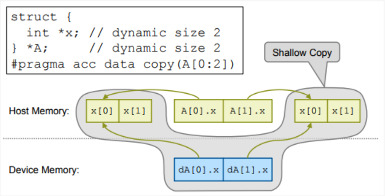


Figure 1. Shallow copy

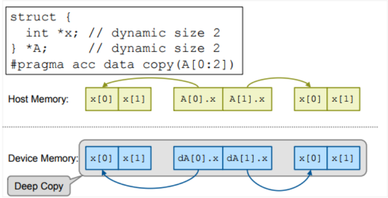


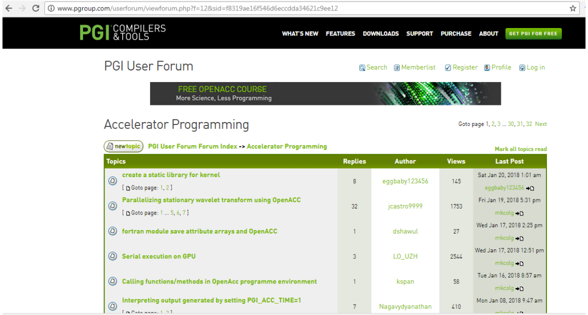
Figure 2. Deep copy

[2]

[2] Beyer, James, David Oehmke, and Jeff Sandoval. "Transferring user-defined types in OpenACC." Proceedings of Cray User Group (2014).

Current limitations (2)

- Debugging is complicated
  - Unsupported use of print functions
- Limited use of dynamic memory in accelerated regions
- Some math library functions are still unsupported
- OpenACC still under development (Compiler Bugs)



Summary

- Minimize data movement
- Maximize compute intensity
- More explicit mapping of parallelism, less portable code
  - Use **device type** clause for architecture-specific optimizations
- When using OpenACC:
  - Measure sequential performance
  - Understand program structure and data movement
  - Find hot-spots (profiler: pgrof, nvvp)
  - Ensure safe parallelism

OpenACC material

Where to find help

- OpenACC Course Recordings - https://developer.nvidia.com/openacc-course
- OpenACC on StackOverflow - http://stackoverflow.com/questions/tagged/openacc
- OpenACC Toolkit - http://developer.nvidia.com/openacc

Additional Resources:

- Parallel Forall Blog - http://devblogs.nvidia.com/parallelforall/
- GPU Technology Conference - http://www.gputechconf.com/
- OpenACC Website - http://openacc.org/

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