CUDA

Operaciones Atómicas

```
x++;
```

read-modify-write operation

1. Read the value in x.
2. Add 1 to the value read in step 1.
3. Write the result back to x.

Condición de carrera

Uno puede tener como resultado 9 u 8

Estaría bueno que exista algo que impida este comportamiento. Estas justamente son las operaciones atómicas. Si un hilo está empleando un valor, traba esa variable para los demás hilos hasta que se deje de usar. Esto se debe hacer con cuidado porque puede romper el paralelismo

Table 9.2 Two threads incrementing the value in x

STEP	EXAMPLE
1. Thread A reads the value in x.	A reads 7 from x.
2. Thread A adds 1 to the value it read.	A computes 8.
3. Thread A writes the result back to x.	x <- 8.
4. Thread B reads the value in x.	B reads 8 from x.
5. Thread B adds 1 to the value it read.	B computes 9.
6. Thread B writes the result back to x.	x <- 9.

Table 9.3 Two threads incrementing the value in x with interleaved operations

STEP	EXAMPLE
Thread A reads the value in x.	A reads 7 from x.
Thread B reads the value in x.	B reads 7 from x.
Thread A adds 1 to the value it read.	A computes 8.
Thread B adds 1 to the value it read.	B computes 8.
Thread A writes the result back to x.	x <- 8.
Thread B writes the result back to x.	x <- 8.

https://docs.nvidia.com/cuda/cuda-c-programming-guide/index.html#atomic-functions

Read-Modify-Write aritmética o lógica en memoria global o compartida

An atomic function performs a read-modify-write atomic operation on one 32-bit or 64-bit word residing in global or shared memory. In the case of `float2` or `float4`, the read-modify-write operation is performed on each element of the vector residing in global memory. For example, `atomicAdd()` reads a word at some address in global or shared memory, adds a number to it, and writes the result back to the same address. Atomic functions can only be used in device functions.

The atomic functions described in this section have ordering cuda::memory_order_relaxed and are only atomic at a particular scope:

- Atomic APIs with `_system` suffix (example: `__atomicAdd_system`) are atomic at scope `cuda::thread_scope_system`.
- Atomic APIs without a suffix (example: `__atomicAdd`) are atomic at scope `cuda::thread_scope_device`.
- Atomic APIs with `_block` suffix (example: `__atomicAdd_block`) are atomic at scope `cuda::thread_scope_block`.

```
int atomicAdd(int* address, int val);
unsigned int atomicAdd(unsigned int* address,
                       unsigned int val);
unsigned long long int atomicAdd(unsigned long long int* address,
                                 unsigned long long int val);
float atomicAdd(float* address, float val);
double atomicAdd(double* address, double val);
__half2 atomicAdd(__half2 *address, __half2 val);
__half atomicAdd(__half *address, __half val);
__nv_bfloat162 atomicAdd(__nv_bfloat162 *address, __nv_bfloat162 val);
__nv_bfloat16 atomicAdd(__nv_bfloat16 *address, __nv_bfloat16 val);
float2 atomicAdd(float2* address, float2 val);
float4 atomicAdd(float4* address, float4 val);
```

reads the 16-bit, 32-bit or 64-bit `old` located at the address `address` in global or shared memory, computes `(old + val)`, and stores the result back to memory at the same address. These three operations are performed in one atomic transaction. The function returns `old`.

Manos a la obra

/share/apps/icnpg/clases/Cuda_Basico/atomics/

ICNPG_atomicas.ipynb

- histograma.cu
- histograma.py
- histograma_thrust_sin_atomics.cu
- reduccion.cu


NVIDIA
CUDA

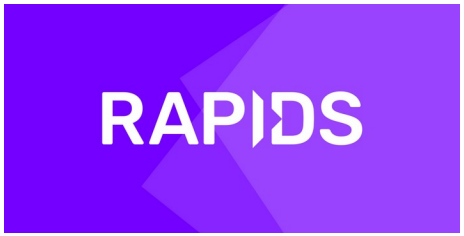

Thrust


Numba
Numba for CUDA GPUs


CuPy


CUDA
FORTRAN


OpenACC
Directives for Accelerators


RAPIDS


C++
Standard Parallelism


PyOpenCL

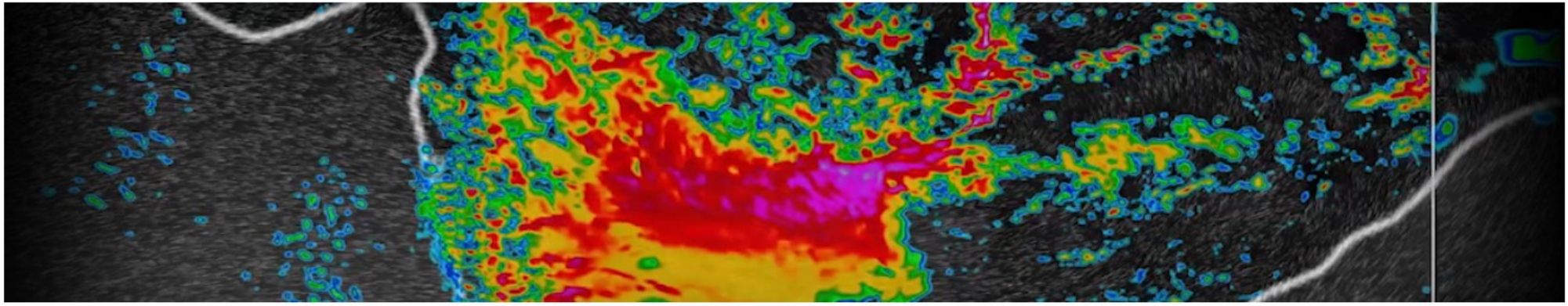

Fortran
Standard Parallelism


julia


SYCL

La magia de los compiladores

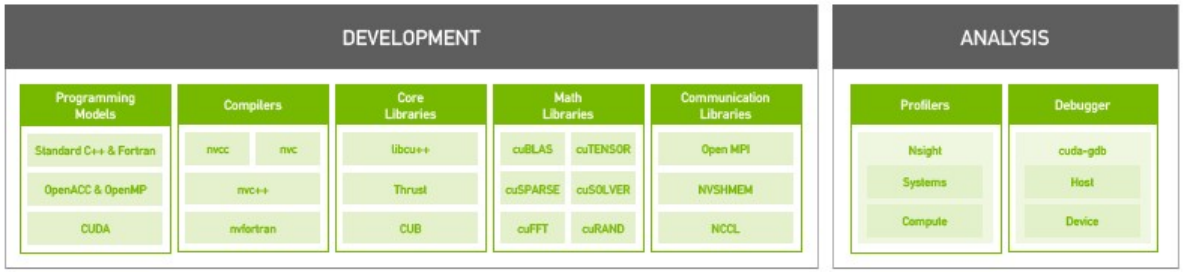
OPENACC



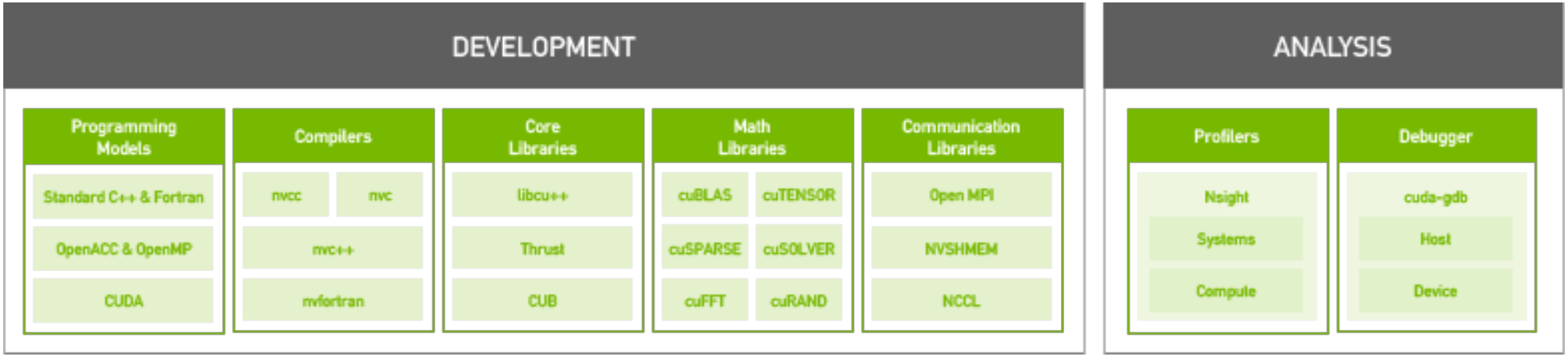
NVIDIA HPC SDK

A Comprehensive Suite of Compilers, Libraries and Tools for HPC

The NVIDIA HPC Software Development Kit (SDK) includes the proven compilers, libraries and software tools essential to maximizing developer productivity and the performance and portability of HPC applications.



https://developer.nvidia.com/hpc-sdk



Compilers

HPC Compilers Documentation
HPC Compiler Documentation Library

nvc
nvc is a C11 compiler for NVIDIA GPUs and AMD, Intel, OpenPOWER, and Arm CPUs. It invokes the C compiler, assembler, and linker for the target processors with options derived from its command line arguments. nvc supports ISO C11, supports GPU programming with OpenACC, and supports multicore CPU programming with OpenACC and OpenMP.

nvc++
nvc++ is a C++17 compiler for NVIDIA GPUs and AMD, Intel, OpenPOWER, and Arm CPUs. It invokes the C++ compiler, assembler, and linker for the target processors with options derived from its command line arguments. nvc++ supports ISO C++17, supports GPU programming with C++17 parallel algorithms (pSTL) and OpenACC, and supports multicore CPU programming with OpenACC and OpenMP.

nvfortran
nvfortran is a Fortran compiler for NVIDIA GPUs and AMD, Intel, OpenPOWER, and Arm CPUs. It invokes the Fortran compiler, assembler, and linker for the target processors with options derived from its command line arguments. nvfortran supports ISO Fortran 2003 and many features of ISO Fortran 2008, supports GPU programming with CUDA Fortran and OpenACC, and supports multicore CPU programming with OpenACC and OpenMP.

nvcc
nvcc is the CUDA C and CUDA C++ compiler driver for NVIDIA GPUs. nvcc accepts a range of conventional compiler options, such as for defining macros and include/library paths, and for steering the compilation process. nvcc produces optimized code for NVIDIA GPUs and drives a supported host compiler for AMD, Intel, OpenPOWER, and Arm CPUs.

Programming Models

C++ Parallel Algorithms
C++ 17 Parallel Algorithms introduce parallel and vector concurrency through execution policies and are supported in the NVC++ compiler.

OpenACC Getting Started Guide
This guide introduces the NVIDIA OpenACC implementation, including examples of how to write, build and run programs using the OpenACC directives.

OpenMP
This section describes using OpenMP, a set of compiler directives, an applications programming interface (API), and a set of environment variables for specifying parallel execution in Fortran, C++ and C programs.

CUDA C++ Programming Guide
A comprehensive guide to understanding and developing and optimizing code in the CUDA C++ programming environment.

CUDA Fortran Programming Guide
This guide describes how to program with CUDA Fortran, a small set of extensions to Fortran that supports and is built upon the NVIDIA CUDA programming model. CUDA Fortran is available on a variety of 64-bit operating systems for both x86 and OpenPOWER hardware platforms. CUDA Fortran includes runtime APIs and programming examples.

¡El compilador se encarga!

DEVELOPER BLOG

This is the first compiler to support GPU-accelerated Standard C++ with no language extensions, pragmas, directives, or non-standard libraries. You can write Standard C++, which is portable to other compilers and systems, and use NVC++ to automatically accelerate it with high-performance NVIDIA GPUs.

HPC Aug 04, 2020

Accelerating Standard C++ with GPUs Using stdpar

By David Olsen, Graham Lopez and Bryce Adelstein Lelbach

Tags: accelerated computing, and compilers, C++, HPC SDK, Languages, programming languages, standard parallelism

Discuss (2)

All data movement between host memory and GPU device memory is performed implicitly and automatically under the control of CUDA Unified Memory.

```
std::sort(employees.begin(), employees.end(),
          CompareByLastName());
```

```
nvc++ -stdpar program.cpp -o program
```

```
std::sort(std::execution::par,
          employees.begin(), employees.end(),
          CompareByLastName());
```

https://developer.nvidia.com/blog/accelerating-standard-c-with-gpus-using-stdpar/

¡El compilador se encarga!

DEVELOPER BLOG

without any extensions, directives, or non-standard libraries.

Fortran
Standard Parallelism

HPC Nov 16, 2020

Accelerating Fortran DO CONCURRENT with GPUs and the NVIDIA HPC SDK

By Guray Ozen and Graham Lopez

Tags: compilers, CUDA, Fortran, HPC SDK, Languages, programming languages, standard parallelism

Discuss (17)

https://developer.nvidia.com/blog/accelerating-fortran-do-concurrent-with-gpus-and-the-nvidia-hpc-sdk/

```
1  subroutine saxpy(x,y,n,a)
2    real :: a, x(:), y(:)
3    integer :: n, i
4    do i = 1, n
5      y(i) = a*x(i)+y(i)
6    enddo
7  end subroutine saxpy
```

```
1  subroutine saxpy(x,y,n,a)
2    real :: a, x(:), y(:)
3    integer :: n, i
4    do concurrent (i = 1: n)
5      y(i) = a*x(i)+y(i)
6    enddo
7  end subroutine saxpy
```

¡El compilador se encarga!

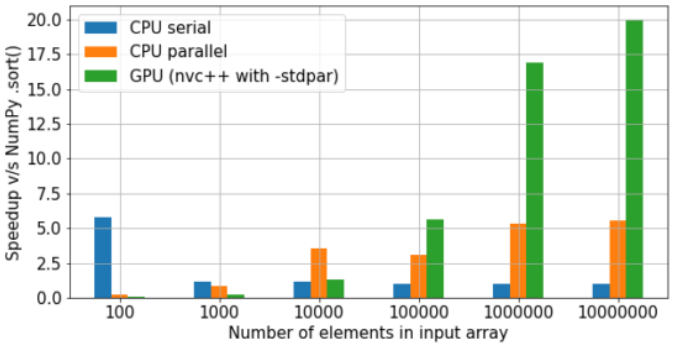


Figure 3. Speedup obtained vs. NumPy for sorting a sequence of integers (larger is better). CPU benchmarks were run on a system with an Intel Xeon Gold 6128 CPU. GPU benchmarks were run on an NVIDIA A100 GPU.

DEVELOPER BLOG

Cython C++ Standard Parallelism

DATA SCIENCE | HPC Nov 10, 2020

Accelerating Python on GPUs with nvc++ and Cython

By Ashwin Srinath

Tags: accelerated computing, Cython, HPC SDK, Python

Discuss (6)

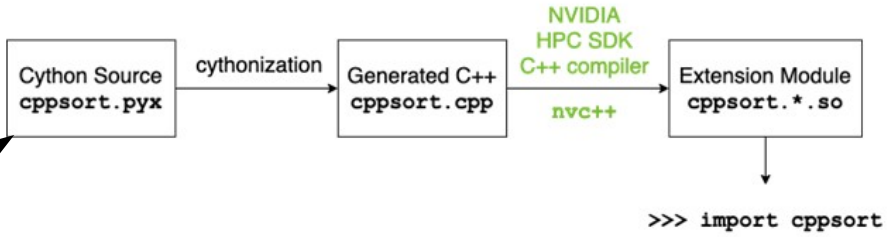


Figure 2. Building an extension module using the nvc++ compiler.

```
from libcpp.algorithm cimport sort, copy_n
from libcpp.vector cimport vector
from libcpp.execution cimport par

def cppsort(int[:] x):
    cdef vector[int] temp
    temp.resize(len(x))
    copy_n(&x[0], len(x), temp.begin())
    sort(par, temp.begin(), temp.end())
    copy_n(temp.begin(), len(x), &x[0])
```

```
In [3]: x = np.array([4, 3, 2, 1], dtype="int32")

In [4]: cppsort(x) # uses the GPU!
```

Key Features

Direct GPU Programming

CUDA Fortran is a low-level explicit programming model with substantial runtime library components that gives expert Fortran programmers direct control over all aspects of GPU programming. CUDA Fortran enables programmers to access and control all the newest GPU features including CUDA Managed Data, Cooperative Groups and Tensor Cores. CUDA Fortran includes several productivity enhancements such as Loop Kernel Directives, module interfaces to the NVIDIA GPU math libraries and OpenACC interoperability features.

CUDA FORTRAN

Host code

```
program t1
use cudafor
use mytests
integer, parameter :: n = 100
integer, allocatable, device :: iarr(:)
integer h(n)
istat = cudaSetDevice(0)
allocate(iarr(n))
h = 0; iarr = h
call test1<<<1,n>>> (iarr)
h = iarr
print *,&
"Errors: ", count(h.ne.(/ (i,i=1,n) /))
deallocate(iarr)
end program t1
```

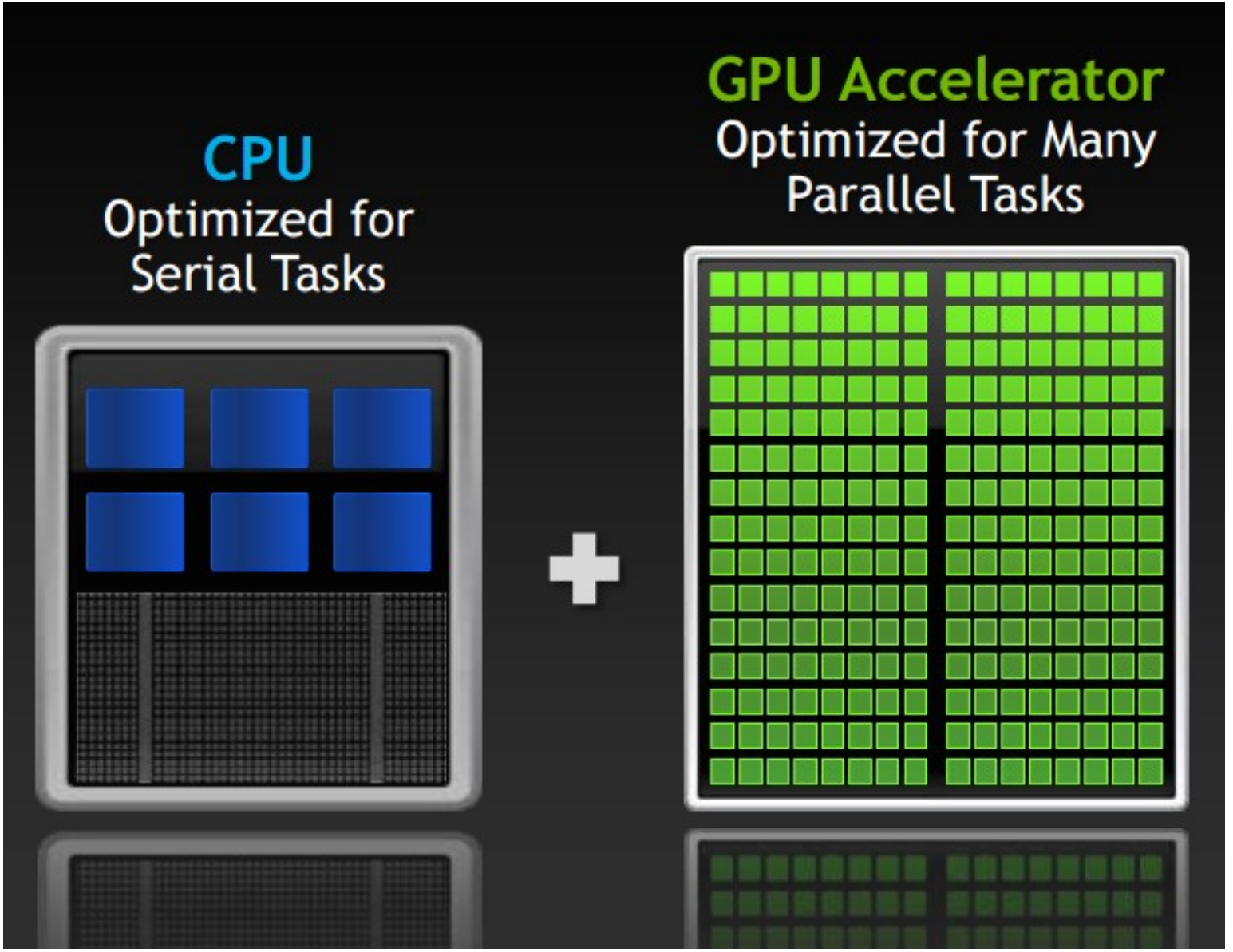
Device Code

```
module mytests
contains
attributes(global)  &
subroutine test1( a )
integer, device :: a(*)
i = threadIdx%x
a(i) = i
return
end subroutine test1
end module mytests
```

```
nvfortran -cuda
```

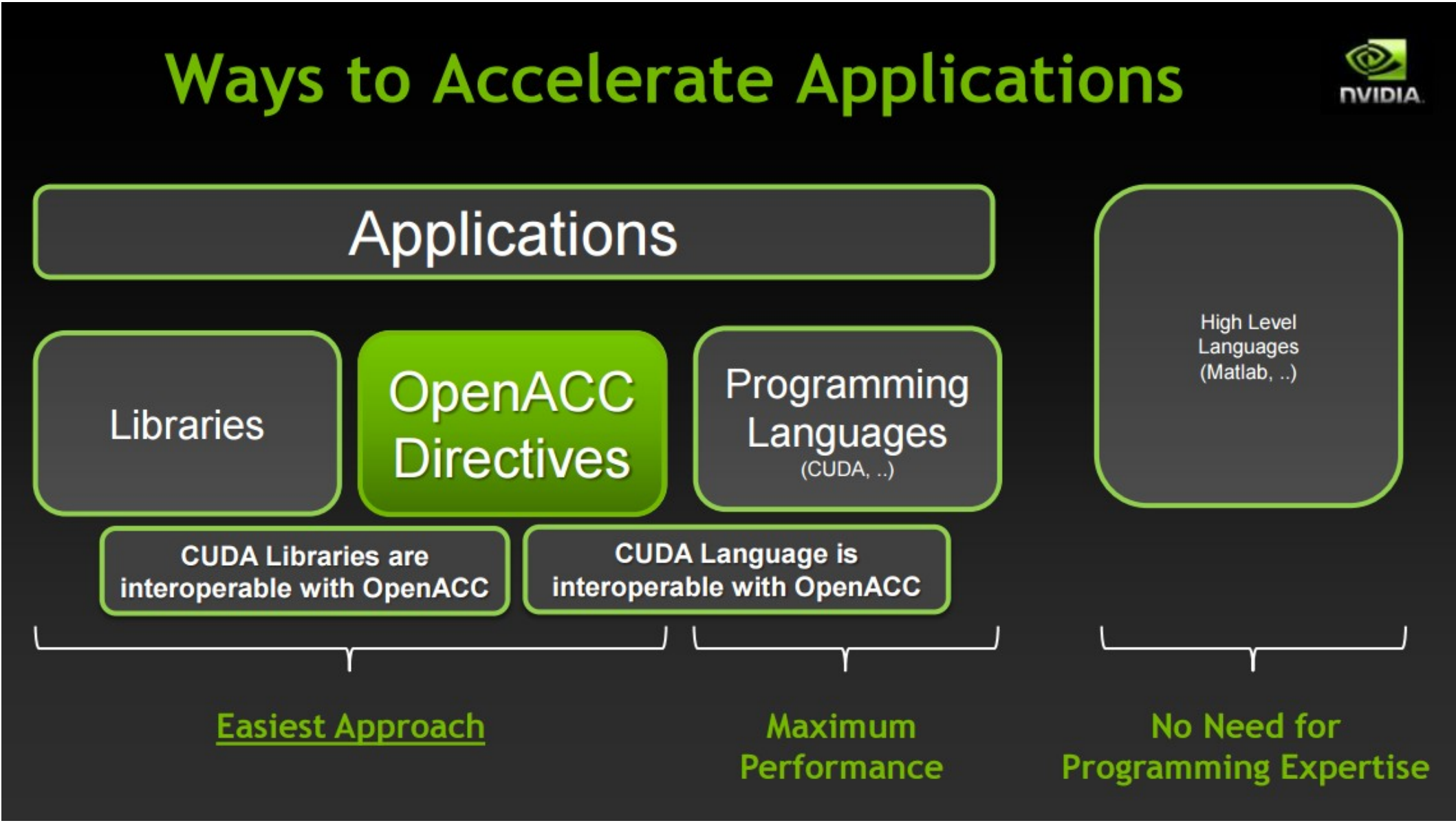
https://docs.nvidia.com/hpc-sdk/compilers/cuda-fortran-prog-guide/index.html

Computación heterogénea



http://lyoncalcul.univ-lyon1.fr/IMG/pdf/00_-_GPU_programming_-_OpenACC_Hands_On.pdf

Otra forma de acelerar aplicaciones ...



http://lyoncalcul.univ-lyon1.fr/IMG/pdf/00_-_GPU_programming_-_OpenACC_Hands_On.pdf

¿ Que es OPENACC ?

http://www.openacc.org/

¿Que es OPENACC?

- Las *directivas* de OpenACC son “hints al compilador” que permiten, sin requerir un nuevo lenguaje como CUDA o OPENCL, acelerar códigos **seriales** en **C/C++ y Fortran** rápidamente en

I. NVIDIA GPUs

II. x86 o ARM CPUs

III. Intel Xeon Phi

IV. AMD Radeon,

- *El compilador se encarga de paralelizar el **código serial**, con ayuda de la información que le damos. Mas allá de eso, delegamos completamente la implementación (muy similar a OPENMP).*

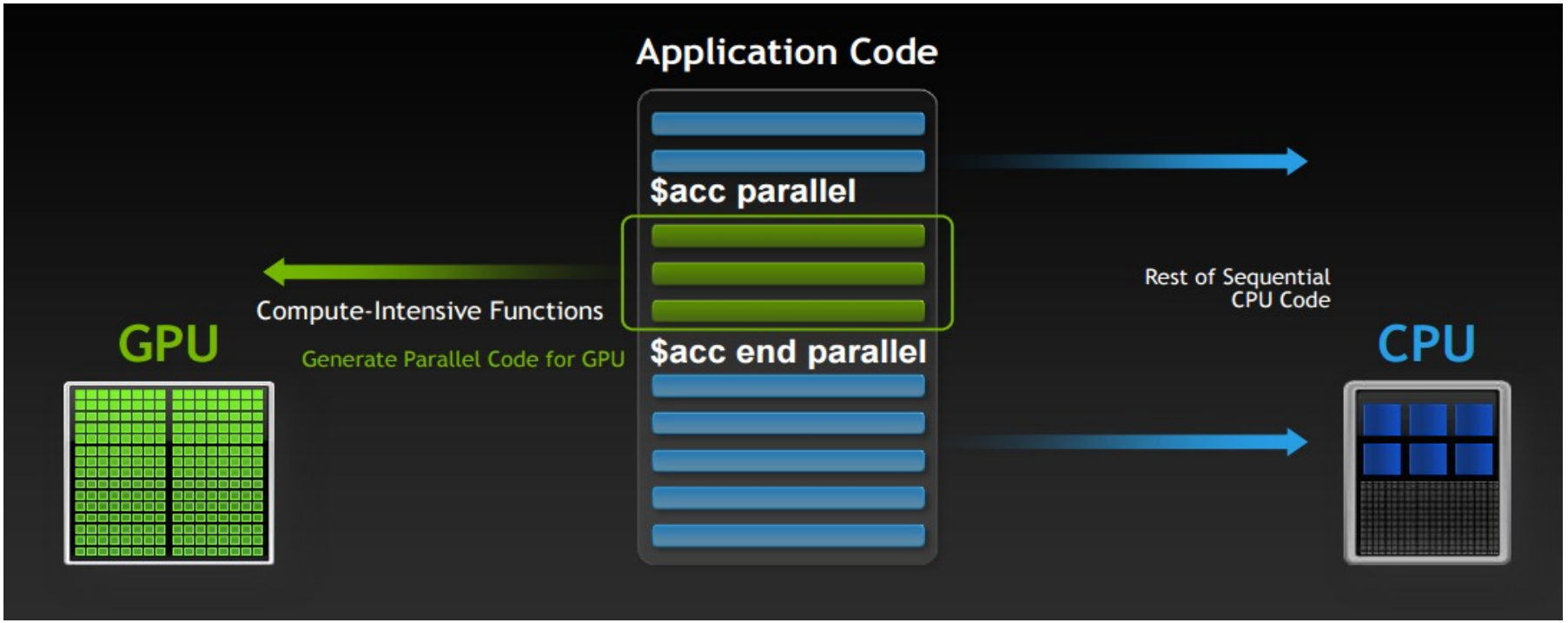
http://www.openacc.org/

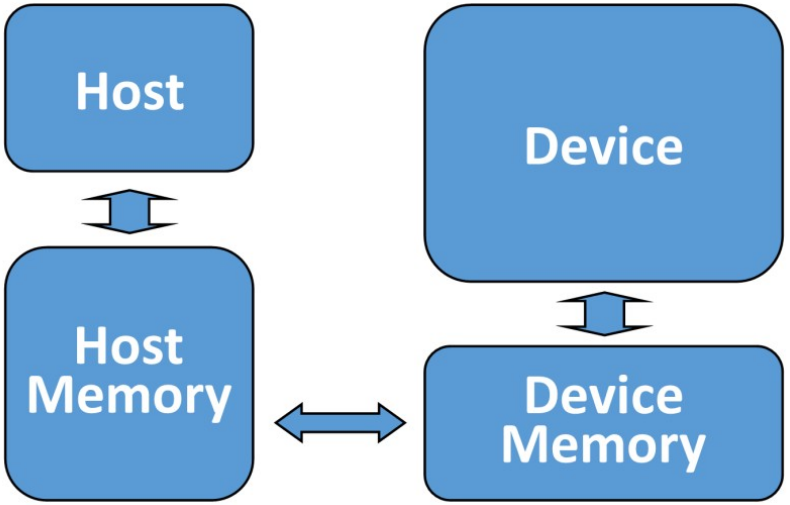
¿Para que sirve OPENACC?

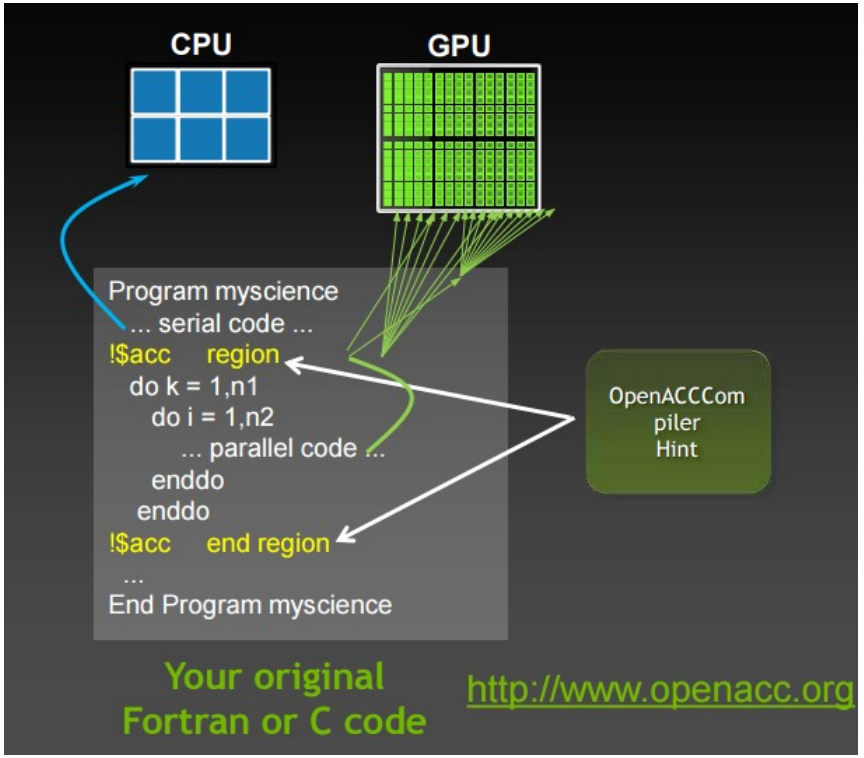
- **Tienen un código serial C/C++/fortran y quieren intentar acelerarlo “rápidamente”:**
  - Modificando mínimamente el código serial original ...
  - Que aún con estas mínimas “adiciones” sea portable y pueda correr normalmente en CPU, como siempre ...
  - Sin necesidad de saber CUDA, OPENCL, OPENMP, etc
  - Sin pretender máxima-performance pero si un mínimo esfuerzo redituable

¿Para quien es OPENACC?

- Heredaste códigos seriales y querés acelerarlos...
- Querés paralelizar pero tenés poco tiempo para programar y/o aprender otro lenguaje
- Querés brindar un “servicio de aceleración” a alguien, sin destruirle el código
- Querés portar a GPU o multicore un software ya hecho (aplicación, librería, etc) con unos mínimos toques...


Application Code
$acc parallel
$acc end parallel
Compute-Intensive Functions
Generate Parallel Code for GPU
GPU
Rest of Sequential
CPU Code
CPU


Host
Host
Memory
Device
Device
Memory


CPU
GPU
Program myscience
... serial code ...
!$acc region
do k = 1,n1
do i = 1,n2
... parallel code ...
enddo
enddo
!$acc end region
...
End Program myscience
OpenACCCom
piler
Hint
Your original
Fortran or C code
http://www.openacc.org

*13x agregando **una sola línea** al programa*

Serial Code

*Single CPU Core Performance: **1x***

```
.
.
.
.
for(int j=1;j<ny-1;j++) {
 for(int k=i1;k<nz-1;k++) {
  for(int i=1;i<nx-1;i++) {
   Anext[Index3D (nx,ny,i,j,k)] =
    (A0[Index3D (nx,ny,i,j,k+1)] +
       A0[Index3D (nx,ny,i,j,k-1)] +
       A0[Index3D (nx,ny,i,j+1,k)] +
       A0[Index3D (nx,ny,i,j-1,k)] +
       A0[Index3D (nx,ny,i+1,j,k)] +
       A0[Index3D (nx,ny,i-1,j,k)])*c1
       -A0[Index3D (nx,ny,i,j,k)]*c0;
   }
  }
}
```

Parallel Code for GPU

Add One OpenACC Directive

*Tesla K40 Perf: **13.6x***

```
.
.
.
#pragma acc parallel loop collapse(3)
for(int j=1;j<ny-1;j++) {
 for(int k=i1;k<nz-1;k++) {
  for(int i=1;i<nx-1;i++) {
   Anext[Index3D (nx,ny,i,j,k)] =
    (A0[Index3D (nx,ny,i,j,k+1)] +
       A0[Index3D (nx,ny,i,j,k-1)] +
       A0[Index3D (nx,ny,i,j+1,k)] +
       A0[Index3D (nx,ny,i,j-1,k)] +
       A0[Index3D (nx,ny,i+1,j,k)] +
       A0[Index3D (nx,ny,i-1,j,k)])*c1
       -A0[Index3D (nx,ny,i,j,k)]*c0;
   }
  }
}
```

Dual socket E5-2698 v3 @2.3GHz (Haswell), 16 cores per socket, 256 GB memory, 1x Tesla K40
Benchmark: Parboil Stencil from University of Illinois with 1000 iterations

Source code for Parboil: http://impact.crhc.illinois.edu/Parboil/parboil.aspx

https://developer.nvidia.com/openacc-toolkit

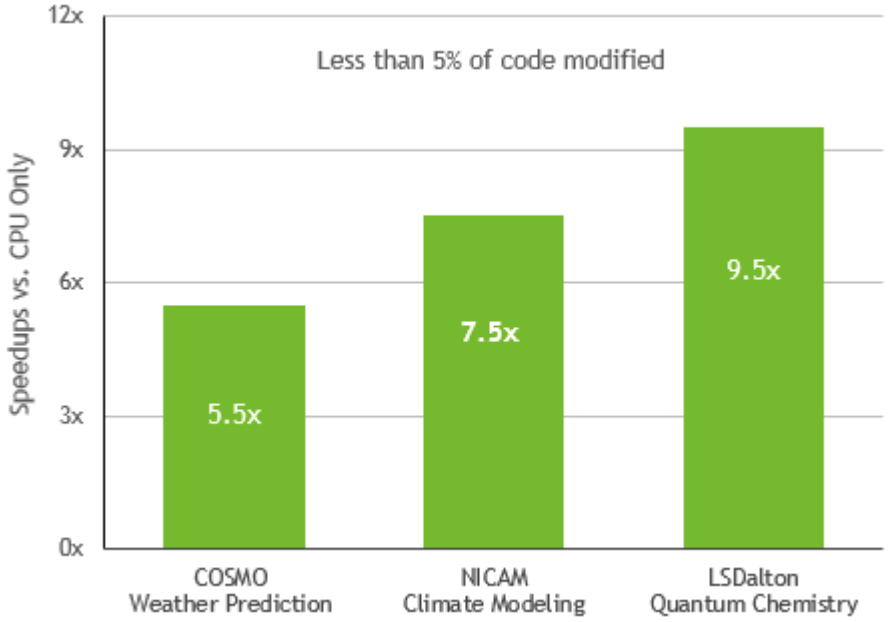
The PGI Community Edition with OpenACC offers scientists and researchers a quick path to accelerated computing with less programming effort. By inserting compiler "hints" or directives into your C, C++ or Fortran code, the PGI OpenACC compiler will offload and run your code on the GPU and CPU.

In addition to the PGI OpenACC compilers, the PGI Community Edition includes GPU-enabled libraries and developer tools to help you with your GPU acceleration effort.

Get Your Free PGI Community Edition Today

DOWNLOAD

- **Simple**: Minimum code modifications to start on GPUs
- **Powerful**: Up to 10x faster application performance
- **Portable**: Same source code runs on CPUs and GPUs

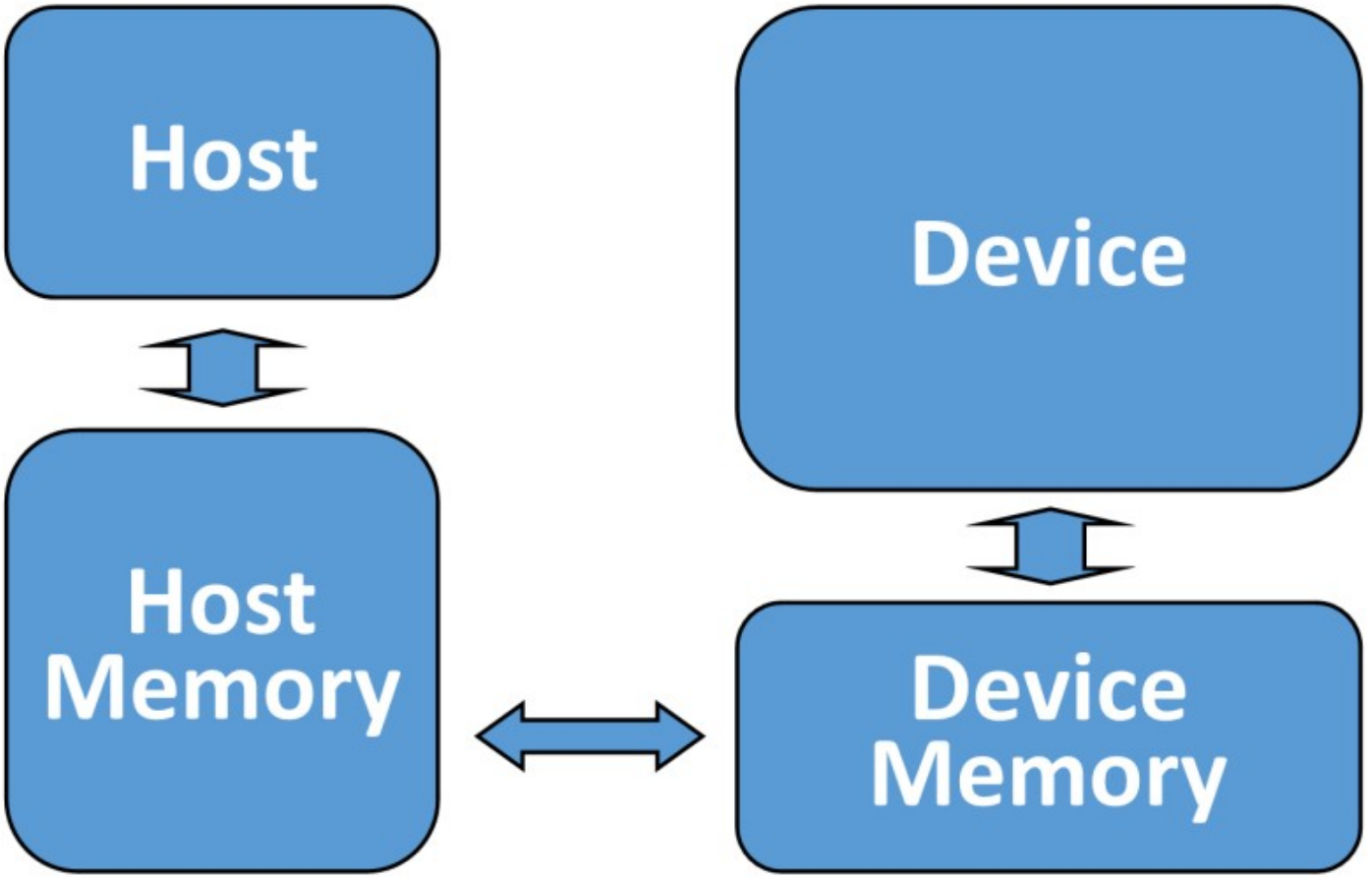


LS-DALTON: Benchmark on Oak Ridge Titan Supercomputer, AMD CPU vs Tesla K20X GPU. Test input: Alanine-3 on CCSD(T) module..

COSMO: additional information here.

NICAM: Benchmark on TiTech TSUBAME 2.5, Westmere CPU vs. K20X, additional information here.

Modelo OPENACC

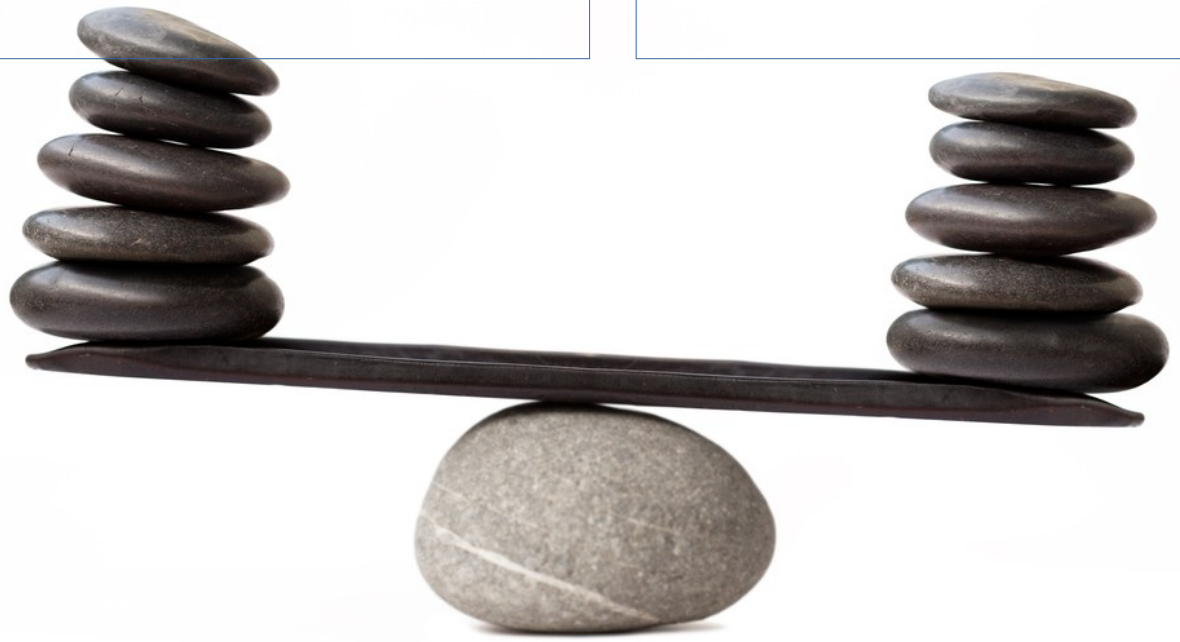


For developers coming to OpenACC from other accelerator programming models, such as CUDA or OpenCL, where host and accelerator memory is frequently represented by two distinct variables (host_A[] and device_A[], for instance), it's important to remember that ***when using OpenACC a variable should be thought of as a single object****, regardless of whether the it's backed by memory in one or more memory spaces.*

Ventajas y desventajas

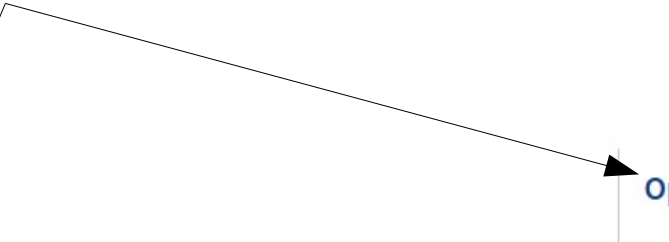
- Muy simple
- Muy Portable
- Fácil de acelerar código serial

- Performance menor a la posible con optimizaciones en CUDA y alguna de sus libs.



La performance puede ser mejorada gracias a su interoperabilidad con CUDA y sus libs, sacrificando portabilidad...

Compiladores



Commercial Compilers

CRAY THE SUPERCOMPUTER COMPANY

Contact Cray Inc for more information.

NVIDIA

NVIDIA HPC SDK. Free download.

国家超级计算无锡中心 National Supercomputing Center in Wuxi

Contact National Supercomputing Center in Wuxi for more information.

Mentor® A Siemens Business

AMD

Sourcery CodeBench (AMD GCN) Lite for X86_64 GNU/Linux

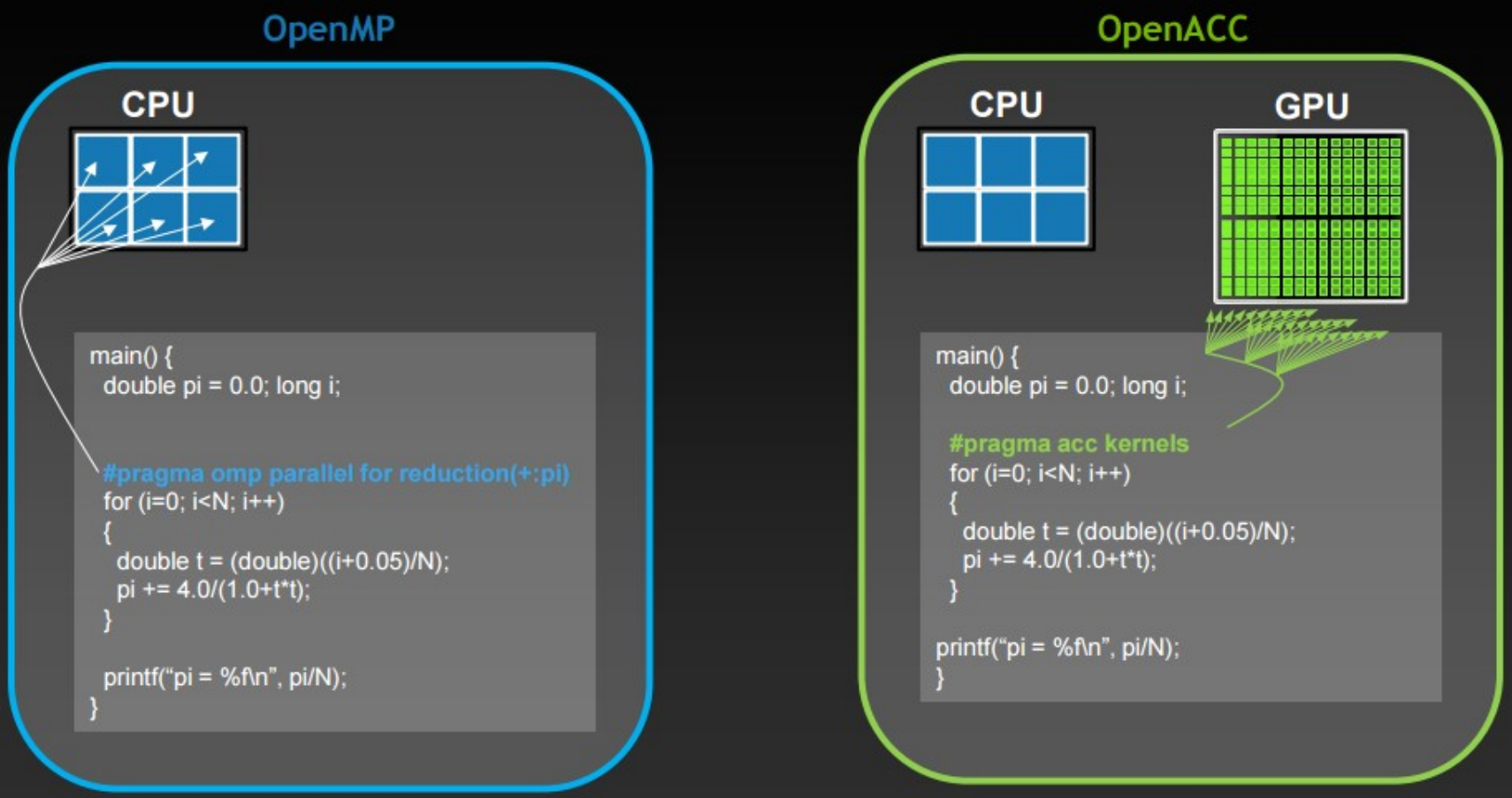
Open Source Compilers

GCC 10

Includes support for OpenACC 2.6

OPENACC y OPENMP

Familiar to OpenMP Programmers



$$\int_0^1 dx \, \frac{4}{1+x^2} = \pi$$

Ecuación de Laplace

- Ecuación de difusión
- Ecuación del calor
- Membrana elástica
- Electrostática...
- Etc.

$$V = f_N(x)$$

$$V = f_O(y)$$

$$(\partial_x^2 + \partial_y^2)V = 0$$

$$V(x,y) = ?$$

$$V = f_E(y)$$

$$V = f_S(x)$$

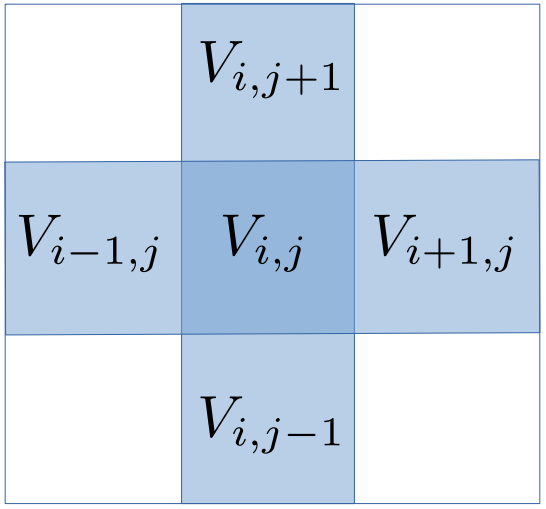
Método de Jacobi

$$(\partial_x^2 + \partial_y^2)V = 0$$

$$V(x = ih, y = jh) = V_{i,j},$$

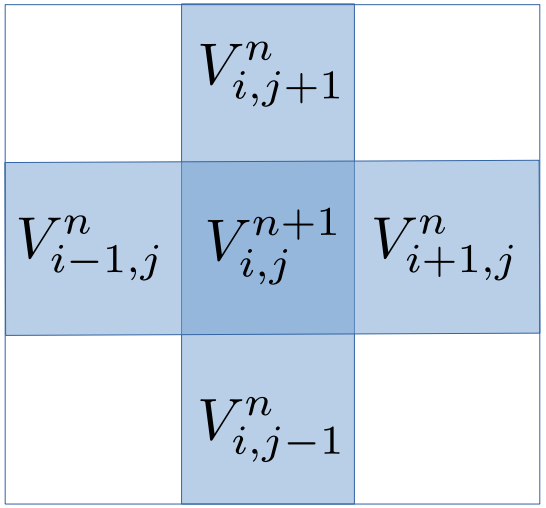
$$V_{i+1,j} + V_{i-1,j} + V_{i,j+1} + V_{i,j-1} - 4V_{i,j} \approx 0$$

$$V_{i,j} \approx \frac{1}{4}(V_{i+1,j} + V_{i-1,j} + V_{i,j+1} + V_{i,j-1})$$



Método de Jacobi

for(n=0....) $$V_{i,j}^{n+1} = \frac{1}{4}(V_{i+1,j}^{n} + V_{i-1,j}^{n} + V_{i,j+1}^{n} + V_{i,j-1}^{n})$$

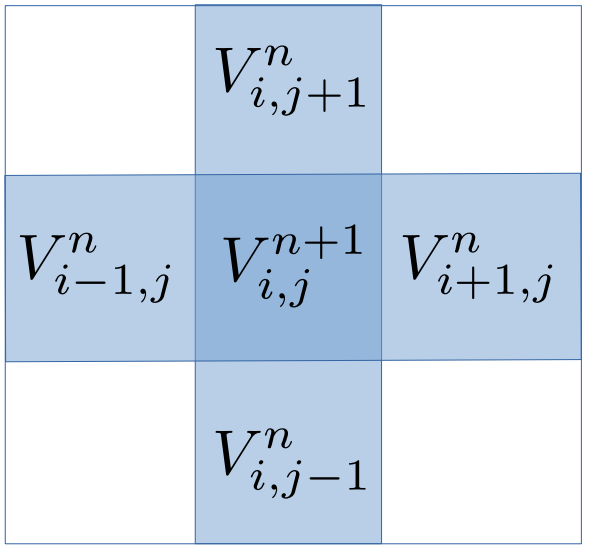


Se puede demostrar que converge a una única solución cuando $n \to \infty$

$$V_{i,j}^{*} = \frac{1}{4}(V_{i+1,j}^{*} + V_{i-1,j}^{*} + V_{i,j+1}^{*} + V_{i,j-1}^{*}) \Rightarrow [\partial_x^2 + \partial_y^2]V^{*}(x,y) = 0$$

Método de Jacobi

$$V_{i,j}^{n+1} = \frac{1}{4}(V_{i+1,j}^{n} + V_{i-1,j}^{n} + V_{i,j+1}^{n} + V_{i,j-1}^{n})$$

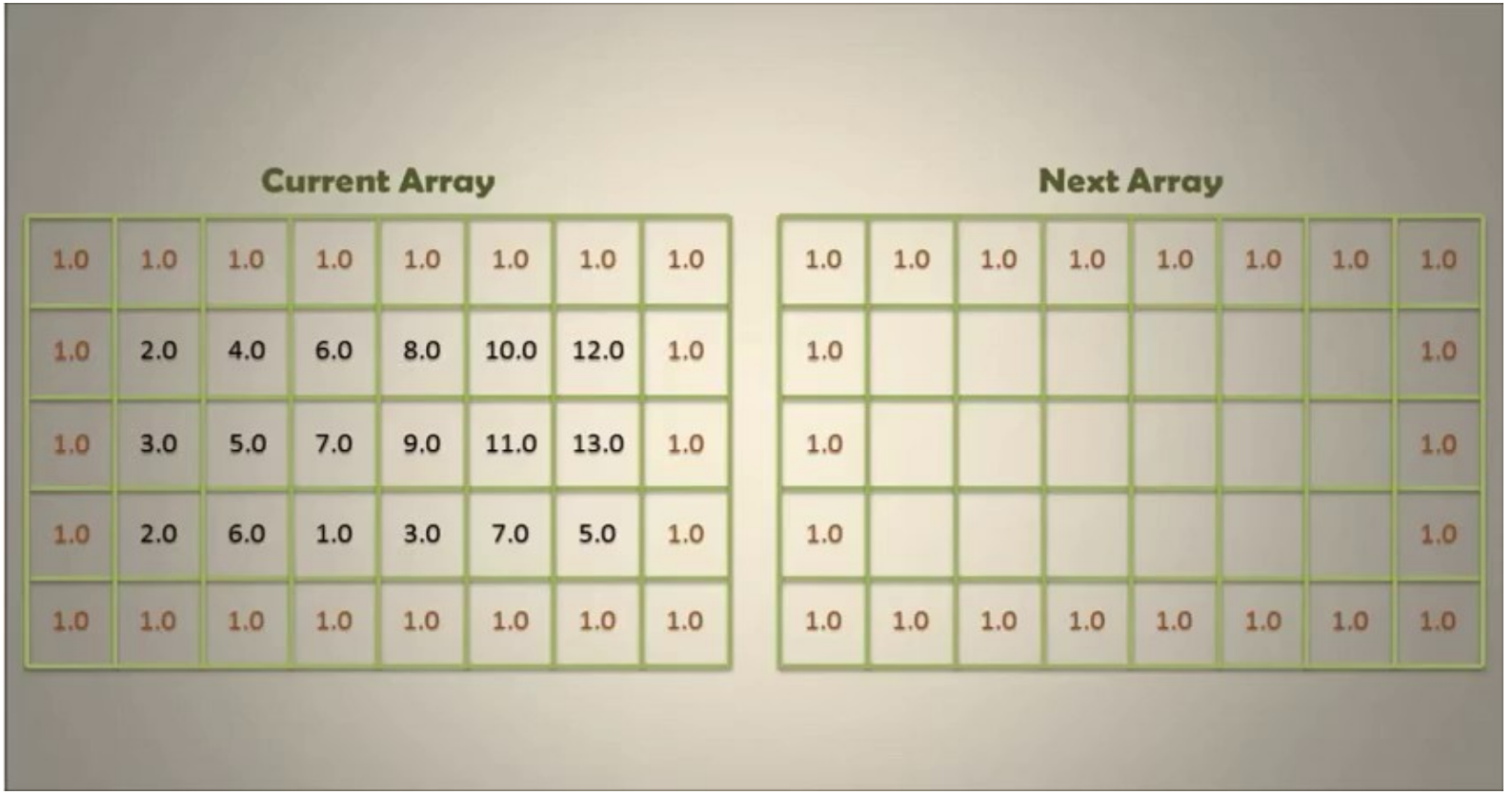


$$\partial_t V = [\partial_x^2 + \partial_y^2]V \Rightarrow V_{i,j}^{n+1} = V_{i,j}^{n} + \frac{\Delta t}{h^2}[V_{i+1,j}^{n} + V_{i-1,j}^{n} + V_{i,j+1}^{n} + V_{i,j+1}^{n} - 4V_{i,j}^{n})]$$

$$\Delta t/h^2 = 1/4 \rightarrow V_{i,j}^{n+1} = V_{i+1,j}^{n} + V_{i-1,j}^{n} + V_{i,j+1}^{n} + V_{i,j-1}^{n}$$

Algoritmo

$$V_{i,j}^{n+1} = \frac{1}{4}(V_{i+1,j}^{n} + V_{i-1,j}^{n} + V_{i,j+1}^{n} + V_{i,j-1}^{n})$$



Programa serial

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

http://lyoncalcul.univ-lyon1.fr/IMG/pdf/00_-_GPU_programming_-_OpenACC_Hands_On.pdf

Programa serial

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

http://lyoncalcul.univ-lyon1.fr/IMG/pdf/00_-_GPU_programming_-_OpenACC_Hands_On.pdf

Manos a la obra...

Manos a la obra...

- **module load nvhpc-21.9**
- **cp -a /share/apps/icnpg/clases/clases_openacc .**
- **cd clases_openacc/jacobi/cudacast**
- Version serial: laplace2d.c
  - **CPU-seq: g++ laplace2d_serial.c -o serial.out**
- Versiones OPENACC (todas con **make**)*:*
  - **GPU: pgcc -I. -acc -ta=nvidia -Minfo=accel -o laplace2d_acc laplace2d.c**
  - **CPU-seq: pgcc laplace2d.c -o laplace2d -I.**
  - **CPU-paralela: pgcc -I. -acc -ta=multicore -Minfo=accel -o laplace2d_acc_multicore laplace2d.c**
- **Version OPENMP**
  - **OMP: pgcc -I. -fast -mp -Minfo -o laplace2d_omp laplace2d.c**
- Correr:
  - **qsub JobGPU ./ejecutable**
- Analizar output: *¿Donde se consume casi todo el tiempo de la corrida?*

OPENMP → paralelización CPU multicore

OpenMP C Code

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

#pragma omp parallel for shared(m, n, Anew, A)
  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 omp parallel for shared(m, n, Anew, A)
  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }

  iter++;
}
```

OpenMP Fortran Code

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

!$omp parallel do shared(m,n,Anew,A) reduction(max:err)
  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

!$omp parallel do shared(m,n,Anew,A)
  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
```

→ *Directivas para indicar paralelización de loops en hilos de la CPU*

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OPENMP vs OPENACC

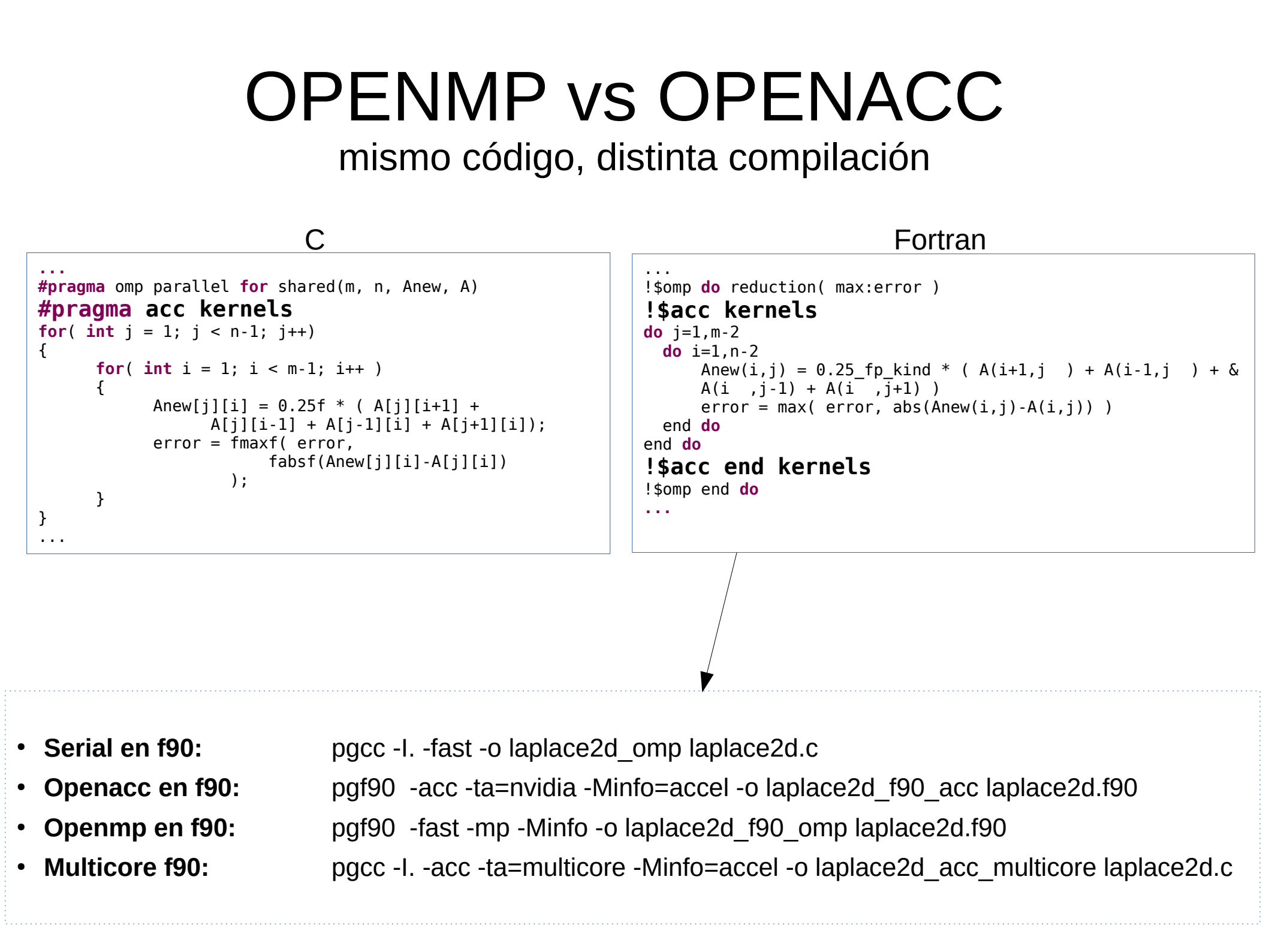
mismo código, distinta compilación

C

```
...
#pragma omp parallel for shared(m, n, Anew, A)
#pragma acc kernels
for( int j = 1; j < n-1; j++)
{
      for( int i = 1; i < m-1; i++ )
      {
            Anew[j][i] = 0.25f * ( A[j][i+1] +
                  A[j][i-1] + A[j-1][i] + A[j+1][i]);
            error = fmaxf( error,
                        fabsf(Anew[j][i]-A[j][i])
                  );
      }
}
...
```

Fortran

```
...
!$omp do reduction( max:error )
!$acc kernels
do j=1,m-2
  do i=1,n-2
      Anew(i,j) = 0.25_fp_kind * ( A(i+1,j  ) + A(i-1,j  ) + &
      A(i  ,j-1) + A(i  ,j+1) )
      error = max( error, abs(Anew(i,j)-A(i,j)) )
  end do
end do
!$acc end kernels
!$omp end do
...
```



- **Serial en f90:** pgcc -I. -fast -o laplace2d_omp laplace2d.c
- **Openacc en f90:** pgf90 -acc -ta=nvidia -Minfo=accel -o laplace2d_f90_acc laplace2d.f90
- **Openmp en f90:** pgf90 -fast -mp -Minfo -o laplace2d_f90_omp laplace2d.f90
- **Multicore f90:** pgcc -I. -acc -ta=multicore -Minfo=accel -o laplace2d_acc_multicore laplace2d.c

Paso 1

- make laplace2d_omp

```
pgcc -I../common -fast -mp -Minfo  -o laplace2d_omp laplace2d.c
main:
    53, Loop not fused: dependence chain to sibling loop
        Generated an alternate version of the loop
        Generated vector sse code for the loop
    59, Loop not fused: function call before adjacent loop
        Generated vector sse code for the loop
    72, Parallel region activated
    80, Parallel loop activated with static block schedule
        Generated an alternate version of the loop
        Generated vector sse code for the loop
    85, Barrier
    87, Parallel region terminated
    88, Parallel region activated
        Parallel loop activated with static block schedule
        Generated vector sse code for the loop
    94, Barrier
        Parallel region terminated
   100, Parallel region activated
        Parallel loop activated with static block schedule
   102, Generated an alternate version of the loop
        Generated vector sse code for the loop
   110, Begin critical section
        End critical section
        Barrier
        Parallel region terminated
   112, Parallel region activated
        Parallel loop activated with static block schedule
   114, Memory copy idiom, loop replaced by call to __c_mcopy4
   120, Barrier
        Parallel region terminated
```

```
#pragma omp parallel shared(Anew)
{
    int tid = omp_get_thread_num();
    if (tid == 0)
    {
            int nthreads = omp_get_num_threads();
            printf("Number of threads = %d\n", nthreads);
    }
#pragma omp parallel for shared(Anew)
    for (int j = 1; j < n; j++)
    {
        Anew[#pragma omp parallel for shared(m, n, Anew, A) reduction(max:error)
        Anew[#pragma acc kernels
    }
                for( int j = 1; j < n-1; j++)
                {
                    for( int i = 1; i < m-1; i++ )
                    {
                        Anew[j][i] = 0.25f * ( A[j][i+1] + A[j][i-1]
                                             + A[j+1][i]);
                        error = max(error, abs(Anew[j][i]-A[j][i]));
#pragma omp parallel for shared(m, n, Anew, A)
#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];
            }
        }

        if(iter % 100 == 0) printf("%5d, %0.6f\n", iter, error);

        iter++;
    }
```

- make laplace2d_acc

```
pgcc -I../common -acc -ta=nvidia,time -Minfo=accel -o laplace2d_acc
laplace2d.c
main:
    99, Generating copyout(Anew[1:4094][1:4094])
        Generating copyin(A[:4096][:4096])
   100, Loop is parallelizable
   102, Loop is parallelizable
```

```
y */
) /* blockIdx.x threadIdx.x */
94])
dx.x */
```

Paso 1

- make laplace2d_omp

```
pgcc -I../common -fast -mp -Minfo  -o laplace2d_omp laplace2d.c
main:
     53,
       C
       C
     59,
       C
     72,
     80,
       C
       C
     85, Barrier
     87, Parallel region termina
     88, Parallel region activat
         Parallel loop activated v
         Generated vector sse c
     94, Barrier
         Parallel region terminat
    100, Parallel region activa
         Parallel loop activated with static block schedule
    102, Generated an alternate version of the loop
         Generated vector sse code for the loop
    110, Begin critical section
         End critical section
         Barrier
         Parallel region terminated
    112, Parallel region activated
         Parallel loop activated with static block schedule
    114, Memory copy idiom, loop replaced by call to __c_mcopy4
    120, Barrier
         Parallel region terminated
```

```
#pragma acc kernels
        for( int j = 1; j < n-1; j++)
        {
            for( int i = 1; i < m-1; i++ )
            {
                Anew[j][i] = 0.25f * ( A[j][i+1] + A[j][i-1]
                                     + A[j-1][i] + A[j+1][i]);
                error = fmaxf( error, fabsf(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];
            }
        }
```

- make laplace2d_acc

```
pgcc -I../common -acc -ta=nvidia,time -Minfo=accel -o laplace2d_acc
laplace2d.c
main:
    99, Generating copyout(Anew[1:4094][1:4094])
        Generating copyin(A[:4096][:4096])
   100, Loop is parallelizable
   102, Loop is parallelizable
        Accelerator kernel generated
        Generating Tesla code
       100, #pragma acc loop gang /* blockIdx.y */
       102, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
       106, Max reduction generated for error
   111, Generating copyin(Anew[1:4094][1:4094])
        Generating copyout(A[1:4094][1:4094])
   112, Loop is parallelizable
   114, Loop is parallelizable
        Accelerator kernel generated
        Generating Tesla code
       112, #pragma acc loop gang /* blockIdx.y */
       114, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
```

Paso 1

Ayúdenme a completar ésta tabla

Ejecución	Tiempo	Aceleración respecto al serial
Serial		
Openmp 2 threads		
Openmp 3 threads		
Openmp 4 threads		
OpenACC		

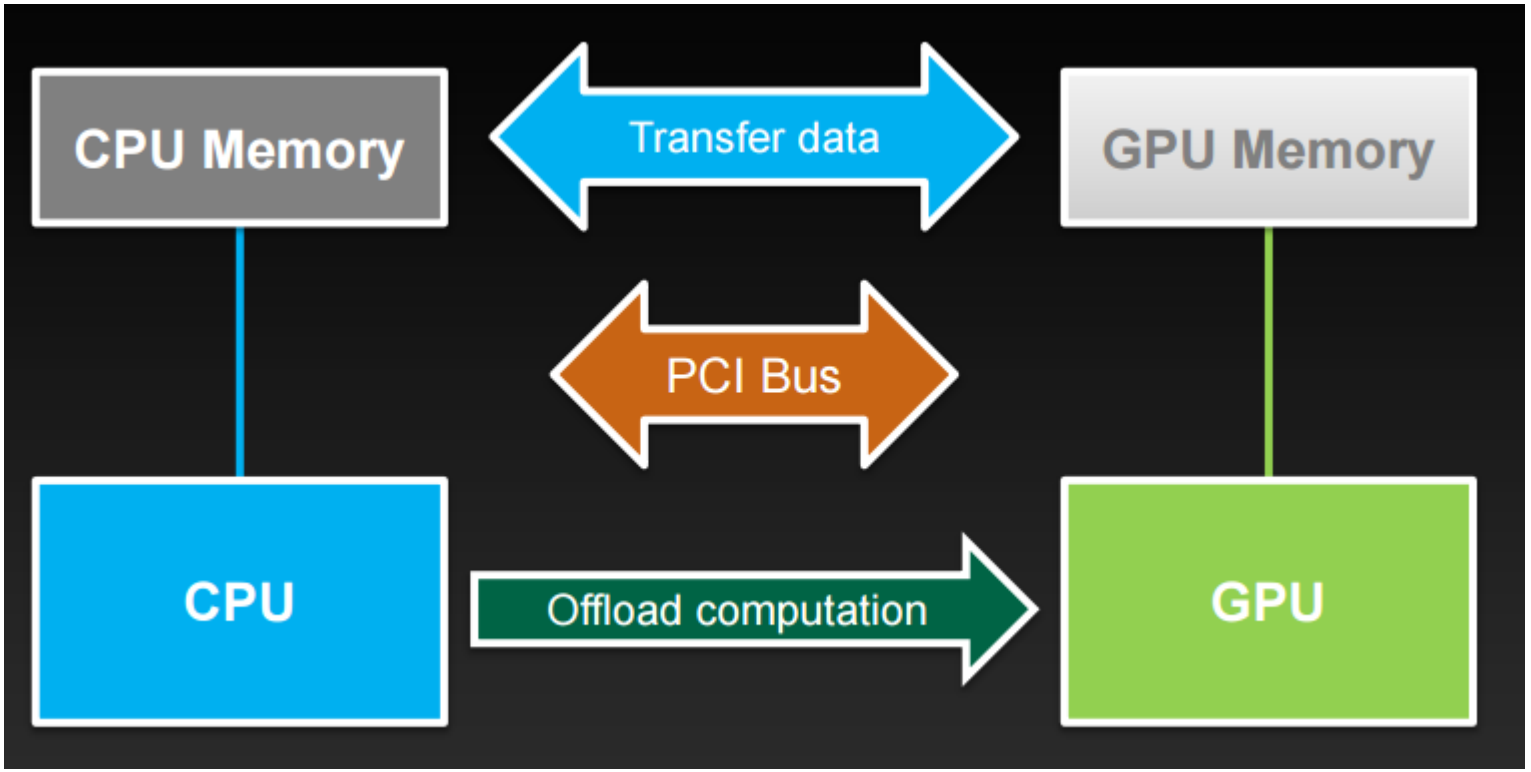
¿Qué paso?

nvprof ./laplace2d_acc

```
==7093== Profiling application: ./laplace2d_acc
==7093== Profiling result:
Time(%)      Time     Calls       Avg       Min       Max  Name
 42.54%  24.2059s      9000  2.6895ms  3.4870us  3.8239ms  [CUDA memcpy
DtoH]
 41.52%  23.6242s      9000  2.6249ms     959ns  3.5642ms  [CUDA memcpy HtoD]
 10.27%  5.84493s      1000  5.8449ms  5.8436ms  5.8544ms  main_102_gpu
  5.20%  2.95895s      1000  2.9590ms  2.9559ms  2.9621ms  main_114_gpu
  0.46%  263.71ms      1000  263.71us  262.65us  265.52us  main_106_gpu_red

==7093== API calls:
Time(%)      Time     Calls       Avg       Min       Max  Name
 98.05%  57.1905s     44996  1.2710ms     404ns  5.8903ms  cuEventSynchronize
```

¡¡¡¡ Excesivo movimiento de datos !!!!!

El precio de transferir...



http://lyoncalcul.univ-lyon1.fr/IMG/pdf/00_-_GPU_programming_-_OpenACC_Hands_On.pdf

CUDA Application Design and Development, R. Farber

THREE RULES OF GPGPU PROGRAMMING

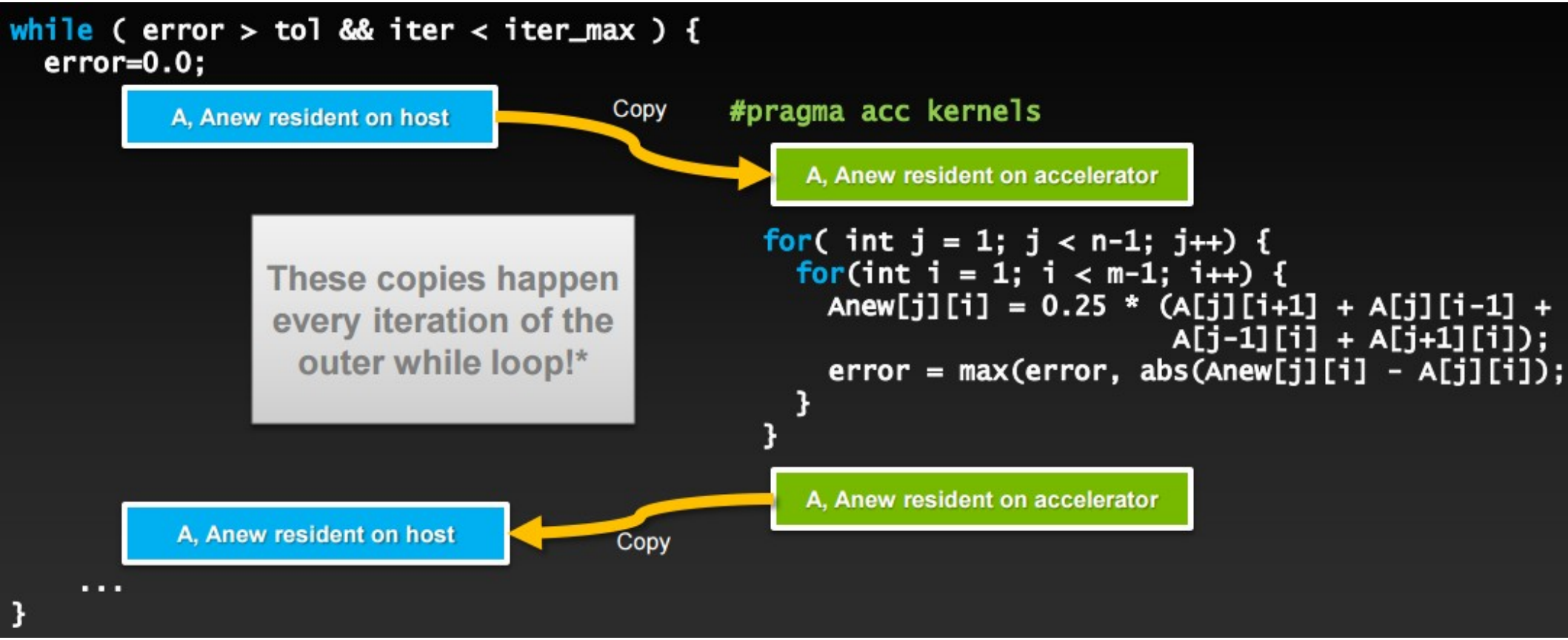
Observation has shown that there are three general rules to creating high-performance GPGPU programs:

1. Get the data on the GPGPU and keep it there.
2. Give the GPGPU enough work to do.
3. Focus on data reuse within the GPGPU to avoid memory bandwidth limitations.

Básicamente es entender las latencias...

¿Compilador precavido o tonto?

*¿Necesitamos **A** y **Anew** en el host cada iteración de Jacobi?*



http://lyoncalcul.univ-lyon1.fr/IMG/pdf/00_-_GPU_programming_-_OpenACC_Hands_On.pdf

¿Compilador precavido o tonto?

*¿Necesitamos **A** y **Anew** en el host cada iteración de Jacobi?*

```
while ( error > tol && iter < iter_max )
    {
        error = 0.f;

#pragma omp parallel for shared(m, n, Anew, A) reduction(max:error)
#pragma acc kernels
        for( int j = 1; j < n-1; j++)
        {
            for( int i = 1; i < m-1; i++ )
            {
                Anew[j][i] = 0.25f * ( A[j][i+1] + A[j][i-1]
                                     + A[j-1][i] + A[j+1][i]);
                error = fmaxf( error, fabsf(Anew[j][i]-A[j][i]));
            }
        }

#pragma omp parallel for shared(m, n, Anew, A)
#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];
            }
        }

        if(iter % 100 == 0) printf("%5d, %0.6f\n", iter, error);

        iter++;
    }
```

¿Que haría Ud aquí si fuera el Compilador?

¿Compilador precavido o tonto?

*¿Necesitamos **A** y **Anew** en el host cada iteración de Jacobi?*

```
do while ( error .gt. tol .and. iter .lt. iter_max )
   error=0.0_fp_kind

!$omp parallel do shared(m, n, Anew, A) reduction( max:error )
!$acc kernels
   do j=1,m-2
     do i=1,n-2
       Anew(i,j) = 0.25_fp_kind * ( A(i+1,j  ) + A(i-1,j  ) + &
                                    A(i  ,j-1) + A(i  ,j+1) )
       error = max( error, abs(Anew(i,j)-A(i,j)) )
     end do
   end do
!$acc end kernels
!$omp end parallel do

   if(mod(iter,100).eq.0 ) write(*,'(i5,f10.6)'), iter, error
   iter = iter +1

!$omp parallel do shared(m, n, Anew, A)
!$acc kernels
   do j=1,m-2
     do i=1,n-2
       A(i,j) = Anew(i,j)
     end do
   end do
!$acc end kernels
!$omp end parallel do

 end do
```

¿Compilador precavido o tonto?

*¿Necesitamos **A** y **Anew** en el host cada iteración de Jacobi?*

```
while ( error > tol && iter < iter_max )
    {
        error = 0.f;

#pragma omp parallel for shared(m, n, Anew, A) reduction(max:error)
#pragma acc kernels
        for( int j = 1; j < n-1; j++)
        {
            for( int i = 1; i < m-1; i++ )
            {
                Anew[j][i] = 0.25f * ( A[j][i+1] + A[j][i-1]
                                     + A[j-1][i] + A[j+1][i]);
                error = fmaxf( error, fabsf(Anew[j][i]-A[j][i]));
            }
        }

#pragma omp parallel for shared(m, n, Anew, A)
#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];
            }
        }

        if(iter % 100 == 0) printf("%5d, %0.6f\n", iter, error);

        iter++;
    }
```

Che, compilador!, **NO** me traigas los datos al host *aquí* porque **no** los voy a necesitar aún!

¿Que haría Ud aquí si fuera el Compilador?

Explotar localidad de Datos

Defining data regions

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

```
!$acc data
    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 data
```

Data Region

Arrays a, b, and c will remain on the GPU until the end of the data region.

http://lyoncalcul.univ-lyon1.fr/IMG/pdf/00_-_GPU_programming_-_OpenACC_Hands_On.pdf

Localidad de los datos

ANTES COPIABAMOS 4 VECES CADA ITERACION

```
while ( error > tol && iter < iter_max )
    {
        error = 0.f;

#pragma omp parallel for shared(m, n, Anew, A)
reduction(max:error)
```

Aquí el compilador copia A, Anew de host a device

```
#pragma acc kernels
        for( int j = 1; j < n-1; j++)
        {
            for( int i = 1; i < m-1; i++ )
            {
                Anew[j][i] = 0.25f * ( A[j][i+1] + A[j][i-1]
                                     + A[j-1][i] + A[j+1][i]);
                error = fmaxf( error, fabsf(Anew[j][i]-A[j][i]));
            }
        }
```

Aquí el compilador, por las dudas, actualiza A, Anew en el host

```
#pragma omp parallel for shared(m, n, Anew, A)
```

Aquí el compilador copia A, Anew de host a device

```
#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];
            }
        }
```

Aquí el compilador, por las dudas, actualiza A, Anew en el host

```
        if(iter % 100 == 0) printf("%5d, %0.6f\n", iter, error);

        iter++;
    }
```

AHORA NOS AHORRAMOS UN MONTON DE COPIAS

Aquí el compilador copia A, Anew al device

```
#pragma acc data copy(A, Anew)
    while ( error > tol && iter < iter_max )
    {
        error = 0.f;

#pragma omp parallel for shared(m, n, Anew, A)
#pragma acc kernels
        for( int j = 1; j < n-1; j++)
        {
            for( int i = 1; i < m-1; i++ )
            {
                Anew[j][i] = 0.25f * ( A[j][i+1] + A[j][i-1]
                                     + A[j-1][i] + A[j+1][i]);
                error = fmaxf( error, fabsf(Anew[j][i]-A[j][i]));
            }
        }
#pragma omp parallel for shared(m, n, Anew, A)
#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];
            }
        }

        if(iter % 100 == 0) printf("%5d, %0.6f\n", iter, error);

        iter++;
    }
```

Recién aquí el compilador actualiza A, Anew en el host como implica el “copy”

Data Regions

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.

http://lyoncalcul.univ-lyon1.fr/IMG/pdf/00_-_GPU_programming_-_OpenACC_Hands_On.pdf

Data Regions

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`.

http://lyoncalcul.univ-lyon1.fr/IMG/pdf/00_-_GPU_programming_-_OpenACC_Hands_On.pdf

Data Regions

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

Data Regions

Update Construct

Fortran

```
!$acc update [clause …]
```

C

```
#pragma acc update [clause …]
```

Clauses

```
host( list )
device( list )
if( expression )
async( expression )
```

Used to update existing data after it has changed in its corresponding copy (e.g. update device copy after host copy changes)

Move data from GPU to host, or host to GPU.
Data movement can be conditional, and asynchronous.

http://lyoncalcul.univ-lyon1.fr/IMG/pdf/00_-_GPU_programming_-_OpenACC_Hands_On.pdf

¿Compilador precavido y/o tonto ?

ANTES

```
while ( error > tol && iter < iter_max )
    {
        error = 0.f;

#pragma omp parallel for shared(m, n, Anew, A)
reduction(max:error)
```

Aquí el compilador copia A, Anew de host a device

```
#pragma acc kernels
        for( int j = 1; j < n-1; j++)
        {
            for( int i = 1; i < m-1; i++ )
            {
                Anew[j][i] = 0.25f * ( A[j][i+1] + A[j][i-1]
                                     + A[j-1][i] + A[j+1][i]);
                error = fmaxf( error, fabsf(Anew[j][i]-A[j][i]));
            }
        }
```

Aquí el compilador, por las dudas, actualiza A, Anew en el host

```
#pragma omp parallel for shared(m, n, Anew, A)
```

Aquí el compilador copia A, Anew de host a device

```
#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];
            }
        }
```

Aquí el compilador, por las dudas, actualiza A, Anew en el host

```
        if(iter % 100 == 0) printf("%5d, %0.6f\n", iter, error);

        iter++;
    }
```

Aquí el compilador copia A, Anew al device

```
#pragma acc data copy(A, Anew)
    while ( error > tol && iter < iter_max )
    {
        error = 0.f;

#pragma omp parallel for shared(m, n, Anew, A)
#pragma acc kernels
        for( int j = 1; j < n-1; j++)
        {
            for( int i = 1; i < m-1; i++ )
            {
                Anew[j][i] = 0.25f * ( A[j][i+1] + A[j][i-1]
                                     + A[j-1][i] + A[j+1][i]);
                error = fmaxf( error, fabsf(Anew[j][i]-A[j][i]));
            }
        }
#pragma omp parallel for shared(m, n, Anew, A)
#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];
            }
        }

        if(iter % 100 == 0) printf("%5d, %0.6f\n", iter, error);

        iter++;
    }
```

Recién aquí el compilador actualiza A, Anew en el host como implica el “copy”

Paso 2

- **Agregar donde corresponda:**
  - **#pragma acc data copy(A), create(Anew)**

Paso 2

Ayudenme de nuevo a completar esta tabla

Ejecución	Tiempo	Aceleración respecto al serial
Serial		
Openmp 2 threads		
Openmp 3 threads		
Openmp 4 threads		
OpenACC		

~15 X

¿Qué paso?

Antes [~150 s, **0.19** x]

```
==7093== Profiling application: ./laplace2d_acc
==7093== Profiling result:
Time(%)      Time     Calls       Avg       Min       Max  Name
 42.54%  24.2059s      9000  2.6895ms  3.4870us  3.8239ms  [CUDA memcpy DtoH]
 41.52%  23.6242s      9000  2.6249ms     959ns  3.5642ms  [CUDA memcpy HtoD]
 10.27%  5.84493s      1000  5.8449ms  5.8436ms  5.8544ms  main_102_gpu
  5.20%  2.95895s      1000  2.9590ms  2.9559ms  2.9621ms  main_114_gpu
  0.46%  263.71ms      1000  263.71us  262.65us  265.52us  main_106_gpu_red

==7093== API calls:
Time(%)      Time     Calls       Avg       Min       Max  Name
 98.05%  57.1905s      44996  1.2710ms     404ns  5.8903ms  cuEventSynchronize
```

Ahora [~4 s, **15** x]

```
==6200== Profiling application: ./laplace2d_acc
==6200== Profiling result:
Time(%)      Time     Calls       Avg       Min       Max  Name
 61.57%  2.36598s      1000  2.3660ms  2.3647ms  2.3704ms  main_94_gpu
 29.62%  1.13818s      1000  1.1382ms  1.1365ms  1.1402ms  main_106_gpu
  7.54%  289.84ms      1000  289.84us  289.09us  290.98us  main_98_gpu_red
  0.70%  26.767ms      1008  26.554us     896ns  3.9257ms  [CUDA memcpy HtoD]
  0.58%  22.279ms      1010  22.058us  2.0800us  2.5660ms  [CUDA memcpy DtoH]

==6200== API calls:
Time(%)      Time     Calls       Avg       Min       Max  Name
 90.78%  3.86609s      5042  766.78us     950ns  3.9326ms  cuEventSynchronize
```

Expresar paralelismo + Explotar localidad de datos =

~15 X

Consejo: 4 pasos

- **Identificar el Paralelismo:**

Mirar, donde el programa pierde mas tiempo, si hay posibilidad de paralelización (loops, loops anidados, etc)

- **Expresar el Paralelismo:**

Poner directivas en los loops para avisarle al compilador donde puede paralelizar. Generalmente da lugar a un código más lento (paso 2)... pero ¡a no desalentarse!.

- **Expresar localidad de datos:**

El compilador no es tan astuto pero es precavido, no puede tomar ciertas decisiones por uno. Decirle entonces como y cuando los datos son necesarios en la GPU o CPU (paso 2).

- **Optimizar:**

Una ayudita extra para mejorar la performance (paso 3), restructurar código o mejorar los patrones de acceso o usar info del hardware... Si no esta satisfecho con las posibilidades que brinda openacc programe la parte crítica en CUDA!, y sacrifique un poco la portabilidad...

https://devblogs.nvidia.com/parallelforall/getting-started-openacc/

Openacc API

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

http://lyoncalcul.univ-lyon1.fr/IMG/pdf/00_-_GPU_programming_-_OpenACC_Hands_On.pdf

Openacc API

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

Kernels Construct

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

```
#pragma acc data copy(A, Anew)
    while ( error > tol && iter < iter_max )
    {
        error = 0.f;

#pragma acc kernels
        for( int j = 1; j < n-1; j++)
        {
            for( int i = 1; i < m-1; i++ )
            {
                Anew[j][i] = 0.25f * ( A[j][i+1] + A[j][i-
1]
                                     + A[j-1][i] + A[j+1]
[i]);
                error = fmaxf( error, fabsf(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];
            }
        }

        if(iter % 100 == 0) printf("%5d, %0.6f\n", iter,
error);

        iter++;
    }
```

http://lyoncalcul.univ-lyon1.fr/IMG/pdf/00_-_GPU_programming_-_OpenACC_Hands_On.pdf

Openacc API

Loop Construct

Fortran

```
!$acc loop [clause …]
    loop
!$acc end loop
```

C

```
#pragma acc loop [clause …]
    { loop }
```

Combined directives

```
!$acc parallel loop [clause …]
!$acc kernels loop [clause …]
```

```
!$acc parallel loop [clause …]
!$acc kernels loop [clause …]
```

Detailed control of the parallel execution of the following loop.

Loop Clauses Inside parallel Region

`gang`	Shares iterations across the gangs of the parallel region.
`worker`	Shares iterations across the workers of the gang.
`vector`	Execute the iterations in SIMD mode.

Loop Clauses

`collapse( n )`	Applies directive to the following `n` nested loops.
`seq`	Executes the loop sequentially on the GPU.
`private( list )`	A copy of each variable in list is created for each iteration of the loop.
`reduction( operator:list )`	`private` variables combined across iterations.

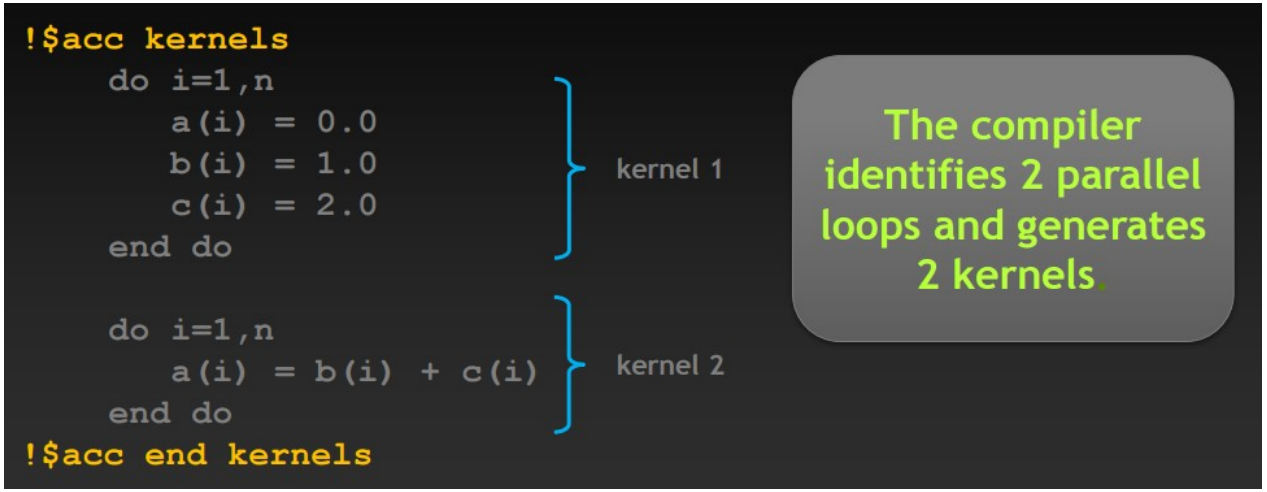
```
#pragma acc data copy(A), create(Anew)
    while ( error > tol && iter < iter_max )
    {
        error = 0.f;

#pragma acc parallel loop collapse(2) reduction(max:error)
        for( int j = 1; j < n-1; j++)
        {
            for( int i = 1; i < m-1; i++ )
            {
                Anew[j][i] = 0.25f * ( A[j][i+1] + A[j][i-1]
                                     + A[j-1][i] + A[j+1][i]);
                error = fmaxf( error, fabsf(Anew[j][i]-A[j][i]));
            }
        }

#pragma acc parallel loop collapse(2)
        for( int j = 1; j < n-1; j++)
        {
            for( int i = 1; i < m-1; i++ )
            {
                A[j][i] = Anew[j][i];
            }
        }

        if(iter % 100 == 0) printf("%5d, %0.6f\n", iter, error);

        iter++;
    }
```

http://lyoncalcul.univ-lyon1.fr/IMG/pdf/00_-_GPU_programming_-_OpenACC_Hands_On.pdf

¿Parallel o Kernel?

- **Parallel**
  - Prescriptivo (como openmp)
  - Usa un kernel en la región
  - El compilador va a acelerar la región *aun si da resultados incorrectos*
  - *Mayor control*
- **Kernels**
  - Descriptivo
  - Usa uno o mas kernels en la región
  - *Más seguro*: podría no acelerar nada si hay ambiguedad
  - *Mejor para empezar* a explorar paralelismo

Ambos definen regiones a ser aceleradas, pero la obligación al compilador es diferente



Se trata de agregar #pragma ...

!$acc kernels	!$acc parallel	!$acc data	!$acc loop	!$acc wait
#pragma acc kernels	#pragma acc parallel	#pragma acc data	#pragma acc loop	#pragma acc wait
Clauses	**Clauses**	**Clauses**	**Clauses**	
if()	if()	if()	collapse()	
async()	async()	async()	within kernels region	
copy()	num_gangs()		gang()	
copyin()	num_workers()		worker()	
copyout()	vector_length()		vector()	
create()	reduction()		seq()	
present()	copyin()	copyin()	private()	
present_or_copy()	copyout()	copyout()	reduction()	
present_or_copyin()	create()	create()		
present_or_copyout()	present()	present()		
present_or_create()	present_or_copy()	deviceptr() in .c		
deviceptr()	present_or_copyin()	deviceptr() in .f		
	present_or_copyout()			
	present_or_create()			
	deviceptr()			
	private()			
	firstprivate()			

```
#pragma acc data copy(A), create(Anew)
    while ( error > tol && iter < iter_max )
    {
        error = 0.f;

#pragma acc parallel loop collapse(2) reduction(max:error)
        for( int j = 1; j < n-1; j++)
        {
            for( int i = 1; i < m-1; i++ )
            {
                Anew[j][i] = 0.25f * ( A[j][i+1] + A[j][i-1]
                                     + A[j-1][i] + A[j+1][i]);
                error = fmaxf( error, fabsf(Anew[j][i]-A[j][i]));
            }
        }

#pragma acc parallel loop collapse(2)
        for( int j = 1; j < n-1; j++)
        {
            for( int i = 1; i < m-1; i++ )
            {
                A[j][i] = Anew[j][i];
            }
        }

        if(iter % 100 == 0) printf("%5d, %0.6f\n", iter, error);

        iter++;
    }
```

http://www.openacc.org/sites/default/files/

Referencias

http://www.openacc.org/content/education

OpenACC Directives for Accelerators

- OpenACC: Directives for GPUs
- FREE OpenACC Online Course
- Six Ways to SAXPY
- An OpenACC Example (Part I, Part II)

OpenACC using the PGI Compilers

- PGI Accelerator Compilers with OpenACC Getting Started Guide (PDF)
- OpenACC Kernels and Parallel Constructs
- The PGI Accelerator Compilers with OpenACC
- 5X in 5 Hours: Porting a 3D Elastic Wave Simulator using OpenACC
- Understanding the CUDA Data Parallel Threading Model

OpenACC using the Cray Compilers

- A Quick Tour of OpenACC
- OpenACC and the Cray Compilation Environment

Developer Support Forums

- Stackoverflow
- PGI

Seminars & Classes

Europe

- CINECA SCAI
- HLRS
- NVIDIA Europe
- PRACE

North America

- Univ. of Houston
- XSEDE

To add a seminar, email training@openacc.org

Videos

- Introduction to OpenACC
- Unstructured Data Lifetimes in OpenACC 2.0 (CUDAcast)
- C++ Class Management with OpenACC 2.0
- Enabling OpenACC Performance Analysis

Learn More

- Debuggers and Other Tools
- Interoperability with MPI

Consulting & Training Services

- Acceleware
- Applied Parallel Computing
- SagivTech

OpenACC Programming and Best Practices Guide

June 2015

Ejemplo de datos con tiempo de vida estructurado.

```
#pragma acc data copy(A), create(Anew)
    while ( error > tol && iter < iter_max )
    {
        error = 0.f;

#pragma acc parallel loop collapse(2) reduction(max:error)
        for( int j = 1; j < n-1; j++)
        {
            for( int i = 1; i < m-1; i++ )
            {
                Anew[j][i] = 0.25f * ( A[j][i+1] + A[j][i-1]
                                     + A[j-1][i] + A[j+1][i]);
                error = fmaxf( error, fabsf(Anew[j][i]-A[j][i]));
            }
        }

#pragma acc parallel loop collapse(2)
        for( int j = 1; j < n-1; j++)
        {
            for( int i = 1; i < m-1; i++ )
            {
                A[j][i] = Anew[j][i];
            }
        }

        if(iter % 100 == 0) printf("%5d, %0.6f\n", iter, error);

        iter++;
    }
```

A, Anew viven aqui arriba

Datos con “tiempo de vida desestructurado”

```
void jacobi(float A[][4096],float Anew[][4096])
{
       int n = 4096;
       int m = 4096;

       int iter = 0;
       const float tol = 1.0e-5f;
       float error     = 1.0f;
       int iter_max = 1000;

       while ( error > tol && iter < iter_max )
       {
           error = 0.f;
#pragma acc parallel loop collapse(2) reduction(max:error)
present(A, Anew)
           for( int j = 1; j < n-1; j++)
           {
               for( int i = 1; i < m-1; i++ )
               {
                   Anew[j][i] = 0.25f * ( A[j][i+1] + A[j][i-1]
                                        + A[j-1][i] + A[j+1][i]);
                   error = fmaxf( error, fabsf(Anew[j][i]-A[j]
[i]));
               }
           }
#pragma acc parallel loop collapse(2) present(A, Anew)
           for( int j = 1; j < n-1; j++)
           {
               for( int i = 1; i < m-1; i++ )
               {
                   A[j][i] = Anew[j][i];
               }
           }

           if(iter % 100 == 0) printf("%5d, %0.6f\n", iter, error);

           iter++;
       }
}
```

- enter data
- exit data

```
int main(int argc, char** argv)
{
     // declaracion, inicializacion de A, Anew en el host
     // etc
#pragma acc enter data copyin(A[0:n][0:m],Anew[0:n][0:m])
     jacobi(A,Anew);
     otra_funcion_acelerada(A,Anew);
#pragma acc exit data delete(A[0:n][0:m],Anew[0:n][0:m])
      // declaracion, inicializacion de A, Anew en el
host
       // etc
   }
```

https://devblogs.nvidia.com/parallelforall/cudacasts-episode-17-unstructured-data-lifetimes-openacc-2-0/

OpenACC Programming and Best Practices Guide

June 2015

UPDATE DIRECTIVES:
Sincronizan los contenidos de las memorias que uno quiera, cuando uno quiera

```
int main(int argc, char** argv)
 {
      // declaracion, inicializacion de A, Anew en el host
      // etc
#pragma acc enter data copyin(A,Anew)

      jacobi(A,Anew);

      funcion_acelerada(A,Anew);

#pragma acc update self(A)
      funcion_no_acelerada(A);
#pragma acc update device(A)

      otra_funcion_acelerada(A,Anew);

#pragma acc exit data delete(A[0:n]
[0:m],Anew[0:n][0:m])
    // declaracion, inicializacion de A, Anew en el host
       // etc
 }
```

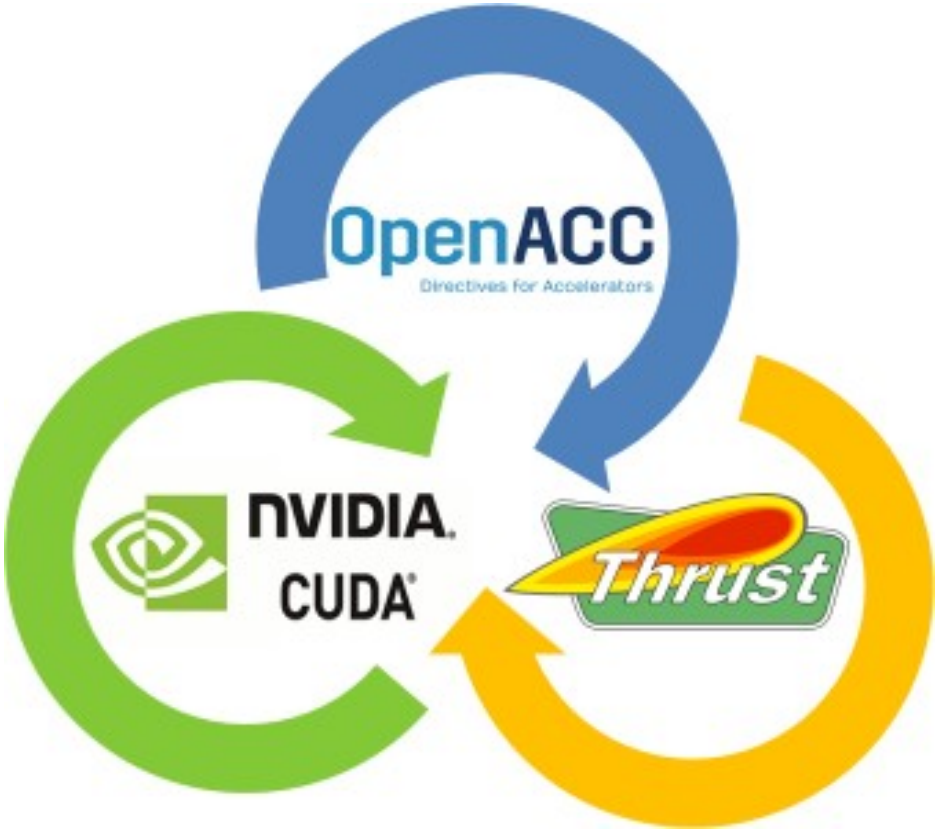
Best Practice: variables in an OpenACC code should always be thought of as a singular object, rather than a host copy and a device copy ….

OPENACC y Template Classes C++

```
template<typename vtype> class myvector
{
          vtype* mydata;
          size_t mysize;
  public:
          inline vtype & operator[]( int i ) const {return mydata[i];}
          inline size_t size(){ return mysize; }
          myvector( int size_ ){
              mysize = size_;
              mydata = new vtype[mysize];
              #pragma acc enter data copyin(this)
              #pragma acc enter data create(mydata[0:mysize])
          }
          ~myvector(){
               #pragma acc exit data delete(mydata[0:mysize],this)
              delete [] mydata;
          }
          void updatedev(){
                 #pragma acc update device(mydata[0:mysize])
          }
          void updatehost(){
                 #pragma acc update host(mydata[0:mysize])
          }
 };
```

```
template<typename vtype> void
    axpy( myvector<vtype>& y, myvector<vtype>& x,
vtype a ){
        #pragma acc parallel loop present(x,y)
        for( int i = 0; i < y.size; ++i )
            y[i] += a*x[i];
    }

template<typename vtype> void
    test( myvector<vtype>& a, myvector<vtype>& b ){
        a.updatedev();
        b.updatedev();
        axpy<vtype>( a, b, 2.0 );
        modify( b );
        b.updatedev();
        axpy<vtype>( a, b, 1.0 );
        a.updatehost();
    }
```

Interoperabilidad



- host_data construct
- deviceptr clause
- acc_map_data() API function.

https://devblogs.nvidia.com/parallelforall/3-versatile-openacc-interoperability-techniques/

Usar CUDA (+libs) en un programa OpenACC con *host_data region*

```
…
#pragma acc data create(x[0:n]) copyout(y[0:n])
{
    #pragma acc kernels
    {
        for( i = 0; i < n; i++){
            x[i] = 1.0f;
            y[i] = 0.0f;
        }
    }
    #pragma acc host_data use_device(x,y)
    {
        cublasSaxpy(n, 2.0, x, 1, y, 1);
    // kernel<<<..,..>>>(x,y,n);
    //
thrust::transform(thrust::device,x,x+n,y,y);
    // etc...
    }
}
...
```

```
program main
  use cublas
  integer, parameter :: N = 2**20
  real, dimension(N) :: X, Y

  !$acc data create(x) copyout(y)

  !$acc kernels
  X(:) = 1.0
  Y(:) = 0.0
  !$acc end kernels

  !$acc host_data use_device(x,y)
  call cublassaxpy(N, 2.0, x, 1, y, 1)
  !$acc end host_data

  !$acc end data

  print *, y(1)
end program
```

The host_data region gives the programmer a way to *expose the device address* of a given array to the host for passing into a function. This data **must have already been moved** to the device previously. The host_data region accepts only the use_device clause, which specifies which device variables should be exposed to the host.

http://www.openacc.org/sites/default/files/

Usar OPENACC en un programa de CUDA con *deviceptr*

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

El array ya esta en device, tomo su puntero...

```
int main(int argc, char **argv)
{
  float *x, *y, tmp;
  int n = 1<<20;

  cudaMalloc((void**)&x,(size_t)n*sizeof(float));
  cudaMalloc((void**)&y,(size_t)n*sizeof(float));

  set(n,1.0f,x);
  set(n,0.0f,y);

  saxpy(n, 2.0, x, y);
  cudaMemcpy(&tmp,y,
(size_t)sizeof(float),cudaMemcpyDeviceToHost);
  printf("%f\n",tmp);
  return 0;
}
```

Usa CUDA API
(podria usar openACC API
o thrust)

In this case OpenACC provides the deviceptr data clause, which may be used where any data clause may appear. This clause informs the compiler that the variables specified are already device on the device and no other action needs to be taken on them.

http://www.openacc.org/sites/default/files/OpenACC_Programming_Guide_0.pdf

Usar OPENACC en un programa de CUDA con *deviceptr*

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

El array ya esta en device, tomo su puntero...

```
int main(int argc, char **argv)
{
      float *x, *y, tmp;
      int n = 1<<20;

      x = acc_malloc((size_t)n*sizeof(float));
      y = acc_malloc((size_t)n*sizeof(float));

      set(n,1.0f,x);
      set(n,0.0f,y);

      saxpy(n, 2.0, x, y);
      acc_memcpy_from_device(&tmp,y,(size_t)sizeof(float));
      printf("%f\n",tmp);
      acc_free(x);
      acc_free(y);
      return 0;
}
```

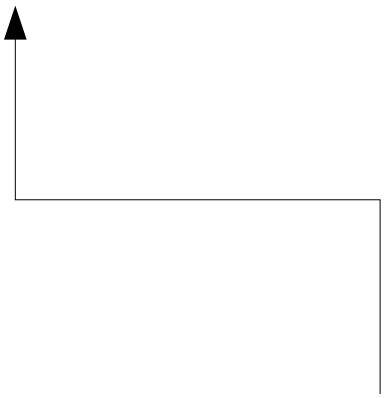
Usa Openacc API
(podria usar CUDA API
o thrust ...)

In this case OpenACC provides the deviceptr data clause, which may be used where any data clause may appear. This clause informs the compiler that the variables specified are already device on the device and no other action needs to be taken on them.

http://www.openacc.org/sites/default/files/OpenACC_Programming_Guide_0.pdf

Usar OPENACC en un programa de Thrust con *deviceptr*

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



```
int main(int argc, char **argv)
{
  int N = 1<<20;
  thrust::host_vector y(N);

  thrust::device_vector d_x(N);
  thrust::device_vector d_y(N);

  thrust::fill(d_x.begin(),d_x.end(), 1.0f);
  thrust::fill(d_y.begin(),d_y.end(), 0.0f);

  saxpy(N, 2.0,
thrust::raw_pointer_cast(d_x.data()),
        thrust::raw_pointer_cast(d_y.data()));

  y = d_y;
  printf("%f\n",y[0]);
  return 0;
}
```

Usar OPENACC en un programa de CUDA con *acc_map_data()*

```
void map(float * restrict harr, float * restrict darr, int size)
{
  acc_map_data(harr, darr, size);
}

void saxpy(int n, float a, float * restrict x, float * restrict y)
{
  // x , y estan presentes en device
  // porque llamamos a acc_map_data()
  #pragma acc kernels present(x,y)
  {
      for(int i=0; i<n; i++)
      {
            y[i] += a*x[i];
      }
  }
}
void set(int n, float val, float * restrict arr)
{
      #pragma acc kernels present(x,y)
      {
            for(int i=0; i<n; i++)
            {
                  arr[i] = val;
            }
      }
}
```

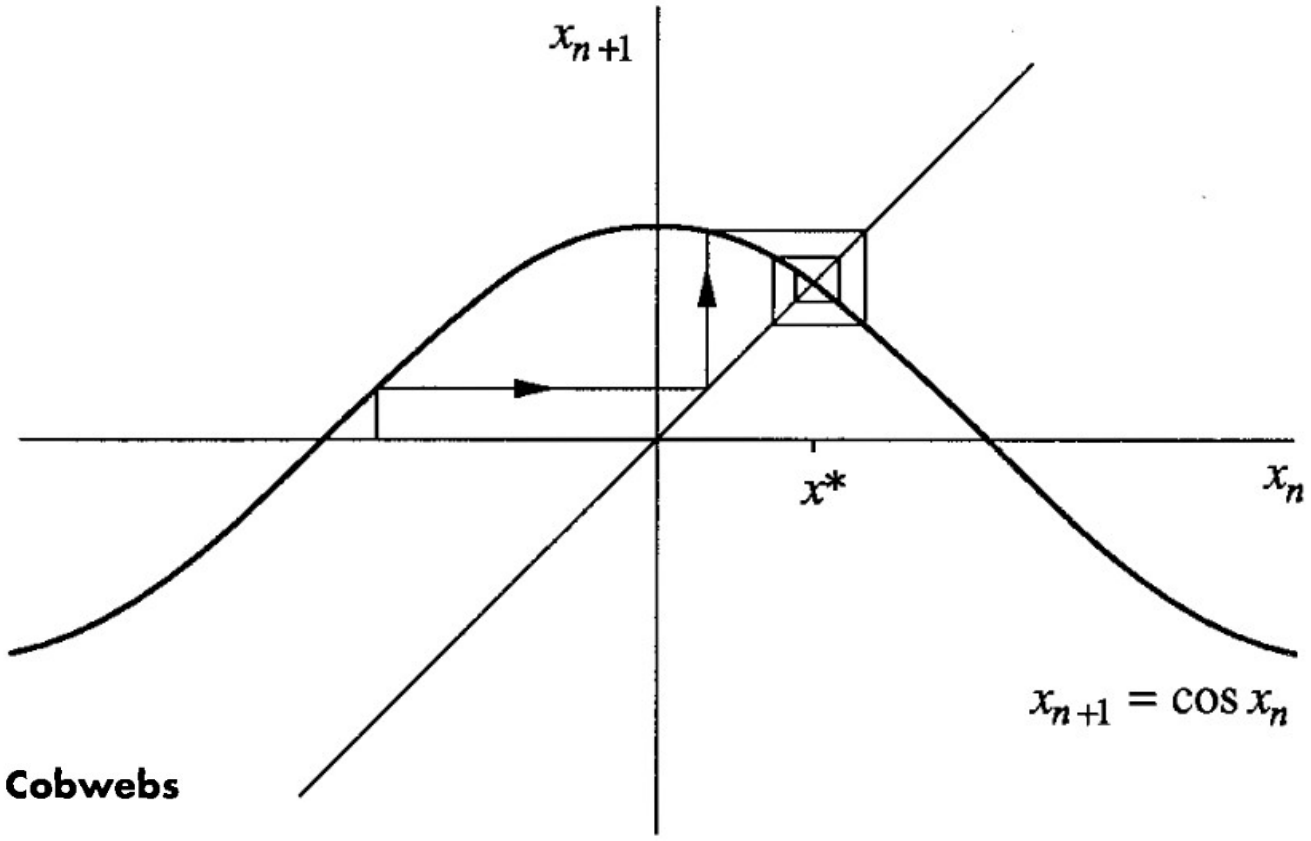
```
int main(int argc, char **argv)
{
  float *x, *y, *dx, *dy, tmp;
  int n = 1<<20;

  x = (float*) malloc(n*sizeof(float));
  y = (float*) malloc(n*sizeof(float));
  cudaMalloc((void**)&dx,(size_t)n*sizeof(float));
  cudaMalloc((void**)&dy,(size_t)n*sizeof(float));

  map(x, dx, n*sizeof(float));
  map(y, dy, n*sizeof(float));

  set(n,1.0f,x);
  set(n,0.0f,y);

  saxpy(n, 2.0, x, y);
  cudaMemcpy(&tmp,dy,
(size_t)sizeof(float),cudaMemcpyDeviceToHost);
  printf("%f\n",tmp);
  return 0;
}
```

The acc_map_data routine is a great way to “set it and forget it” when it comes to sharing memory between CUDA and OpenACC ...

http://www.openacc.org/sites/default/files/OpenACC_Programming_Guide_0.pdf

Mapeos unidimensionales

Given $x_{n+1} = \cos x_n$, how does x_n behave as $n \to \infty$?



Converge a un punto fijo… ¿qué otra cosa puede pasar en general?

Manos a la obra...

- **cd openacc-interoperability**
- **make *nombre_ejemplo***
- **qsub submit_gpu.sh *nombre_ejemplo***

- *nombre_ejemplo* es alguno de estos:
- * **cuda_main** - calling OpenACC from CUDA C
- * **openacc_c_main** - Calling CUDA from OpenACC in C
- * **openacc_c_cublas** - Calling CUBLAS from OpenACC in C
- * **thrust** - Mixing OpenACC and Thrust in C++
- * **cuda_map** - Using OpenACC acc_map_data with CUDA in C
- * **cuf_main** - Calling OpenACC from CUDA Fortran
- * **cuf_openacc_main** - Calling CUDA Fortran from OpenACC
- * **openacc_cublas** - Calling CUBLAS from OpenACC in CUDA Fortran
- * **acc_malloc** - Same as cuda_main, but using the OpenACC API
- * **openacc_streams** - Mixes OpenACC async queues and CUDA streams
- * **openacc_cuda_device** - Calls a CUDA __device__ kernel within an OpenACC
- Author: Jeff Larkin <jlarkin@nvidia.com>

Referencias

- OpenACC Course Recordings - https://developer.nvidia.com/openacc-courses
- PGI Website - http://www.pgroup.com/resources
- OpenACC on StackOverflow - http://stackoverflow.com/questions/tagged/openacc
- OpenACC Toolkit - http://developer.nvidia.com/openacc-toolkit
- Parallel Forall Blog - http://devblogs.nvidia.com/parallelforall/
- GPU Technology Conference - http://www.gputechconf.com/
- OpenACC Website - http://openacc.org/

Openacc + avanzado

- Optimización de loops
- Asincronismo
- Multi GPU

Quizás más adelante....