Towards an integration of directive-based and explicit accelerator programming models

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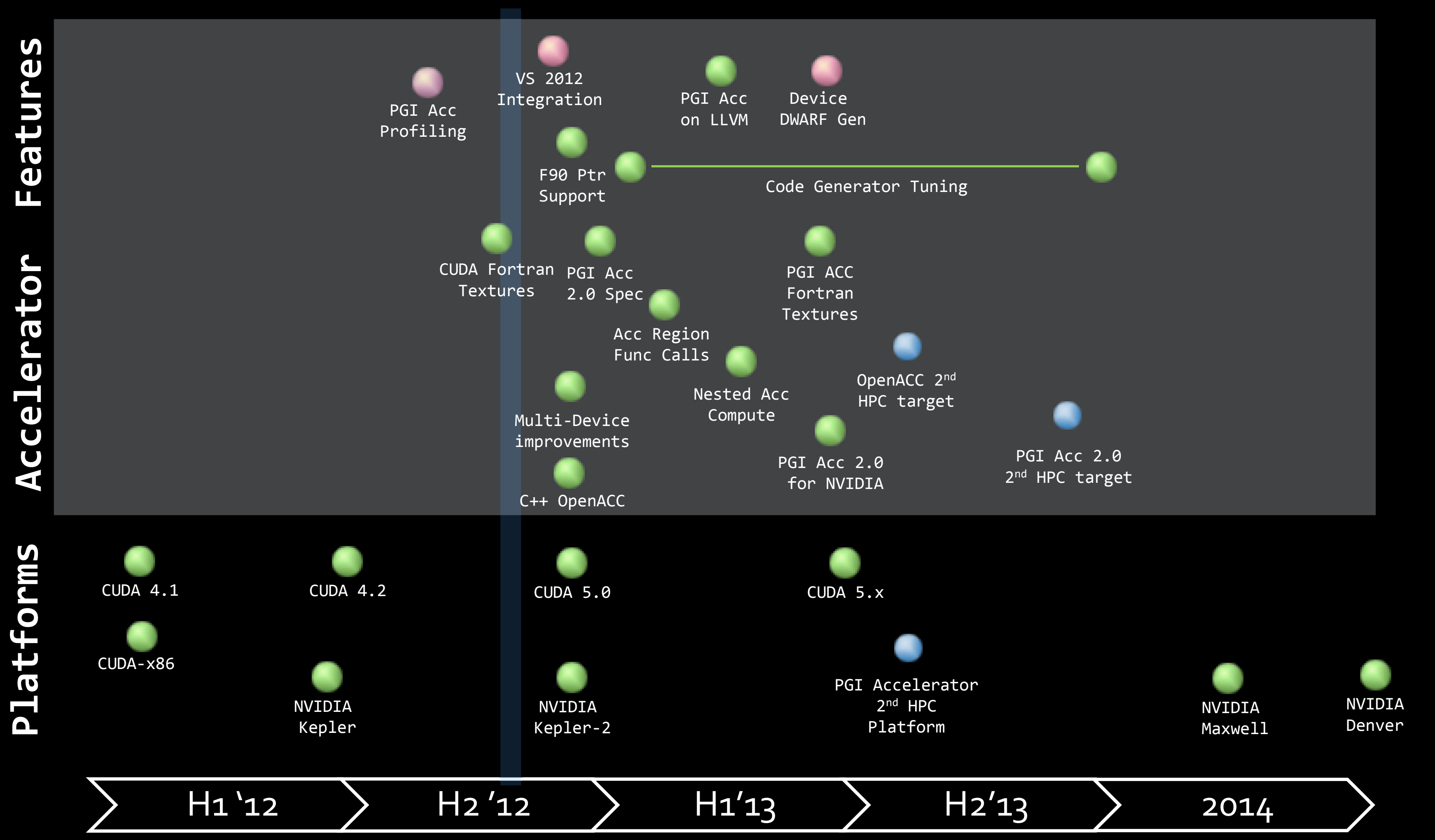
Overview

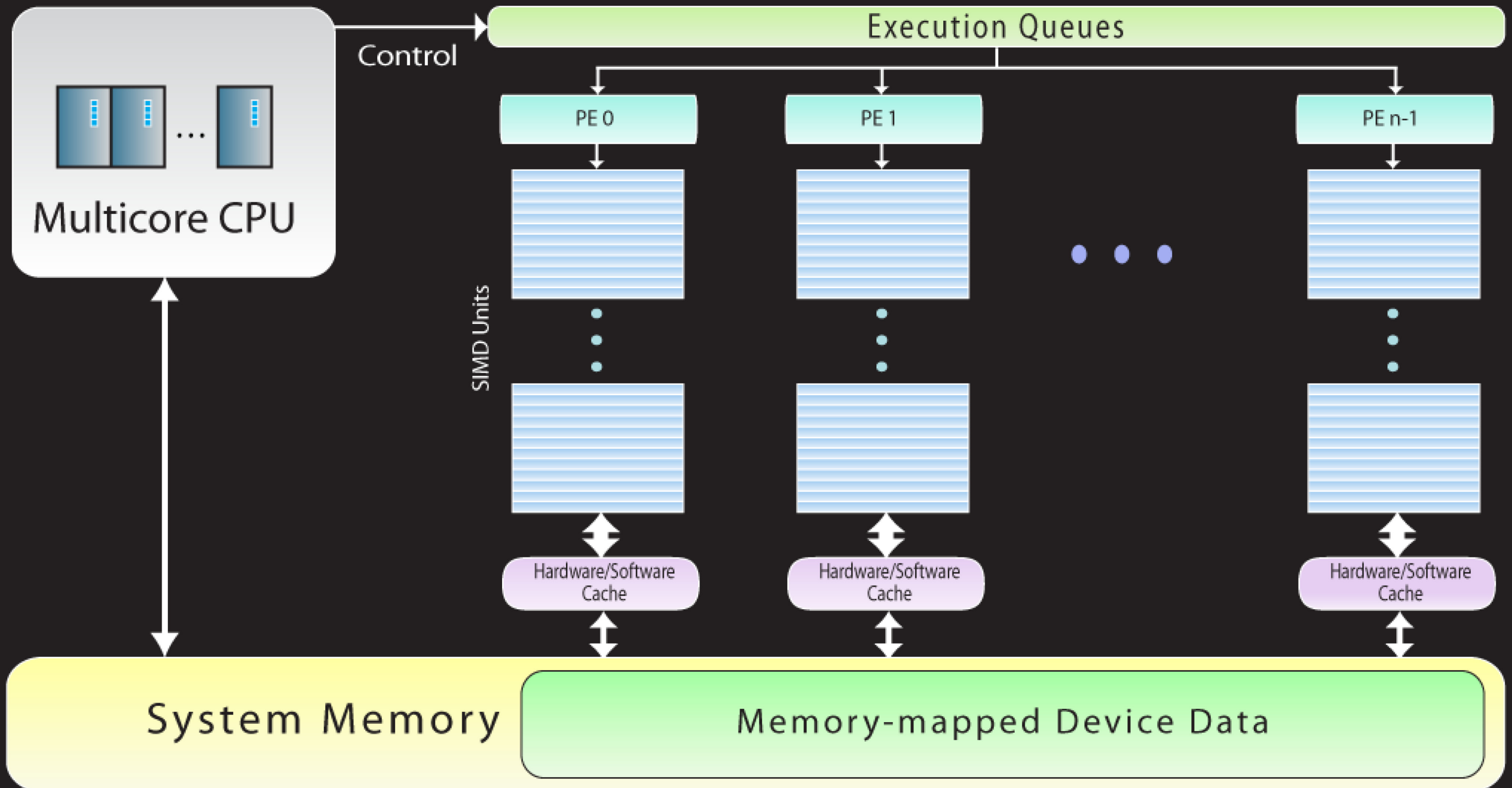
- PGI Accelerator / OpenACC roadmap
- An abstract machine for OpenACC programmers
- Directives are necessary, but are they sufficient?
- What’s so great about CUDA Fortran?
- Elements of an integrated model

PGI Accelerator / OpenACC Roadmap*



*PGI roadmaps are subject to change without notice

OpenACC Abstract Machine Architecture



Directives are necessary, but are they sufficient?

- What about library developers, other experts?
- Accelerator performance cliff
- Predictability
- Compiler maturity
- Portability, OpenACC interoperability of explicit models

What’s so great about CUDA Fortran?

1. The host code – it looks normal!

```
real, device, allocatable, dimension(:,:) ::
        Adev,Bdev,Cdev

. . .

allocate (Adev(N,M), Bdev(M,L), Cdev(N,L))
Adev = A(1:N,1:M)
Bdev = B(1:M,1:L)

call mm_kernel <<<dim3(N/16,M/16),dim3(16,16)>>>
                ( Adev, Bdev, Cdev, N, M, L)

C(1:N,1:L) = Cdev
deallocate ( Adev, Bdev, Cdev )

. . .
```

```
attributes(global) subroutine mm_kernel
              ( A, B, C, N, M, L )
real :: A(N,M), B(M,L), C(N,L), Cij
integer, value :: N, M, L
integer :: i, j, kb, k, tx, ty
real, shared :: Asub(16,16),Bsub(16,16)
tx = threadidx%x
ty = threadidx%y
i = blockidx%x * 16 + tx
j = blockidx%y * 16 + ty
Cij = 0.0
do kb = 1, M, 16
   Asub(tx,ty) = A(i,kb+tx-1)
   Bsub(tx,ty) = B(kb+ty-1,j)
   call syncthreads()
   do k = 1,16
      Cij = Cij + Asub(tx,k) * Bsub(k,ty)
   enddo
   call syncthreads()
enddo
C(i,j) = Cij
end subroutine mmul_kernel
```

CPU Code

GPU Code

2. OpenACC interoperability

```
module mymod
  real, dimension(:), allocatable, device :: xDev
end module
...
use mymod
...
allocate( xDev(n) )
call init_kernel <<<dim3(n/128),dim3(128)>>> (xDev, n)
...
!$acc data copy( y(:) )   ! no need to copy 'xDev'
  ...
!$acc kernels loop
  do i = 1, n
    y(i) = y(i) + a*xDev(i)
  enddo
  ...
!$acc end data
```

3. !$CUF kernel directives

```
module madd_device_module
  use cudafor
contains
  subroutine madd_dev(a,b,c,sum,n1,n2)
    real,dimension(:,:),device :: a,b,c
    real :: sum
    integer :: n1,n2
    type(dim3) :: grid, block
!$cuf kernel do (2) <<<(*,*),(32,4)>>>
    do j = 1,n2
      do i = 1,n1
        a(i,j) = b(i,j) + c(i,j)
        sum = sum + a(i,j)
      enddo
    enddo
  end subroutine
end module
```

Equivalent hand-written CUDA kernels

```
module madd_device_module
  use cudafor
  implicit none
contains
  attributes(global) subroutine madd_kernel(a,b,c,blocksum,n1,n2)
    real, dimension(:,:) :: a,b,c
    real, dimension(:) :: blocksum
    integer, value :: n1,n2
    integer :: i,j,tindex,tneighbor,bindex
    real :: mysum
    real, shared :: bsum(256)
! Do this thread's work
    mysum = 0.0
    do j = threadidx%y + (blockidx%y-1)*blockdim%y, n2, blockdim%y*griddim%y
      do i = threadidx%x + (blockidx%x-1)*blockdim%x, n1, blockdim%x*griddim%x
        a(i,j) = b(i,j) + c(i,j)
        mysum = mysum + a(i,j) ! accumulates partial sum per thread
      enddo
    enddo
! Now add up all partial sums for the whole thread block
! Compute this thread's linear index in the thread block
! We assume 256 threads in the thread block
    tindex = threadidx%x + (threadidx%y-1)*blockdim%x
! Store this thread's partial sum in the shared memory block
    bsum(tindex) = mysum
    call syncthreads()
! Accumulate all the partial sums for this thread block to a single value
    tneighbor = 128
    do while( tneighbor >= 1 )
      if( tindex <= tneighbor ) &
        bsum(tindex) = bsum(tindex) + bsum(tindex+tneighbor)
      tneighbor = tneighbor / 2
      call syncthreads()
    enddo
! Store the partial sum for the thread block
    bindex = blockidx%x + (blockidx%y-1)*griddim%x
    if( tindex == 1 ) blocksum(bindex) = bsum(1)
  end subroutine

! Add up partial sums for all thread blocks to a single cumulative sum
  attributes(global) subroutine madd_sum_kernel(blocksum,dsum,nb)
    real, dimension(:) :: blocksum
    real :: dsum
    integer, value :: nb
    real, shared :: bsum(256)
    integer :: tindex,tneighbor,i
! Again, we assume 256 threads in the thread block
! accumulate a partial sum for each thread
    tindex = threadidx%x
    bsum(tindex) = 0.0
    do i = tindex, nb, blockdim%x
      bsum(tindex) = bsum(tindex) + blocksum(i)
    enddo
    call syncthreads()
! This code is copied from the previous kernel
! Accumulate all the partial sums for this thread block to a single value
! Since there is only one thread block, this single value is the final result
    tneighbor = 128
    do while( tneighbor >= 1 )
      if( tindex <= tneighbor ) &
        bsum(tindex) = bsum(tindex) + bsum(tindex+tneighbor)
      tneighbor = tneighbor / 2
      call syncthreads()
    enddo
    if( tindex == 1 ) dsum = bsum(1)
  end subroutine

  subroutine madd_dev(a,b,c,dsum,n1,n2)
    real, dimension(:,:), device :: a,b,c
    real, device :: dsum
    real, dimension(:), allocatable, device :: blocksum
    integer :: n1,n2,nb
    type(dim3) :: grid, block
    integer :: r
! Compute grid/block size; block size must be 256 threads
    grid = dim3((n1+31)/32, (n2+7)/8, 1)
    block = dim3(32,8,1)
    nb = grid%x * grid%y
    allocate(blocksum(1:nb))
    call madd_kernel<<< grid, block >>>(a,b,c,blocksum,n1,n2)
    call madd_sum_kernel<<< 1, 256 >>>(blocksum,dsum,nb)
    r = cudaThreadSynchronize() ! don't deallocate too early
    deallocate(blocksum)
  end subroutine
end module
```

4. Generic interfaces and overloading

```
use cublas

real(4), device :: xd(N)
real(4) x(N)
call random_number(x)

! On the device
allocate(xd(N))
xd = x
j = isamax(N,xd,1)

! On the host, same name
k = isamax(N,x,1)
```

```
module cublas
! isamax
  interface isamax
    integer function isamax &
       (n, x, incx)
    integer :: n, incx
    real(4) :: x(*)
    end function

    integer function isamaxcu &
       (n, x, incx) bind(c, &
            name='cublasIsamax')
    integer, value :: n, incx
    real(4), device :: x(*)
    end function
  end interface
. . .
```

5. Encapsulation

- Isolate device data and accelerator kernel declarations in Fortran modules

```
module mm
    real, device, allocatable :: a(:)
    real, device :: x, y(10)
    real, constant :: c1, c2(10)
    integer, device :: n
  contains
    attributes(global) subroutine s( b )
  ...
```

- Partition source into sections written and maintained by accelerator experts versus those evolved by science and engineering domain experts

Elements of an integrated model

- Execution model – host-directed execution with one or more attached accelerator devices
- Memory model – allow for separated host & device memories, an exposed device memory hierarchy
- Portable high-level programming with OpenACC directives
- Portable low-level programming based loosely on CUDA and OpenCL

New low-level procedure attributes

- Host proc's in C/C++: `__host__ int func(…)`
  Fortran: `attributes(host) subroutine(…)`

- Kernel proc's in C/C++: `__kernel__ void func(…)`
  Fortran: `attributes(kernel) subroutine(…)`

- Device proc's in C/C++: `__device__ int func(…)`
  Fortran: `attributes(device) subroutine(…)`

New low-level variable attributes

- Host data (default)
- Device data in C/C++: `__device__`, `__deviceptr__`
  Fortran: `attributes(device)`
- Constant data in C/C++: `__constant__`
  Fortran: `attributes(constant)`
- Shared data in C/C++: `__shared__`
  Fortran: `attributes(shared)`
- Pinned data in C/C++: `__pinned__`
  Fortran: `attributes(pinned)`

Portable low-level API functions

- Device mgmt – acc_get_num_devices, acc_set_device_type, acc_get_device_type, acc_get_device_num, acc_set_device_num, acc_init, acc_shutdown

- Memory mgmt – acc_malloc, acc_free, acc_memset, acc_memset_async, acc_memcpy_to_device, acc_memcpy_to_device_async , acc_memcpy_to_host, acc_memcpy_to_host_async, … error handling, etc

- Asynchronous execution mgmt – acc_async_test, acc_async_test_all, acc_async_wait, acc_async_wait_all, … event mgmt?

… You get the idea

PGI Accelerator C++ 2.0?

WARNING – Slideware Alert!

```
__deviceptr__ float *adev, *bdev, *cdev;
. . .
adev = new float[n*m];
bdev = new float[m*l];
cdev = new float[n*l];

adev[0:n*m] = a[0:n*m];
bdev[0:m*l] = b[0:m*l];

mm_kernel <<<dim3(n/16,m/16),dim3(16,16)>>>
          ( adev, bdev, cdev, n, m, l);

c[0:n*l] = cdev[0:n*l];
delete [] adev, bdev, cdev;
. . .
```

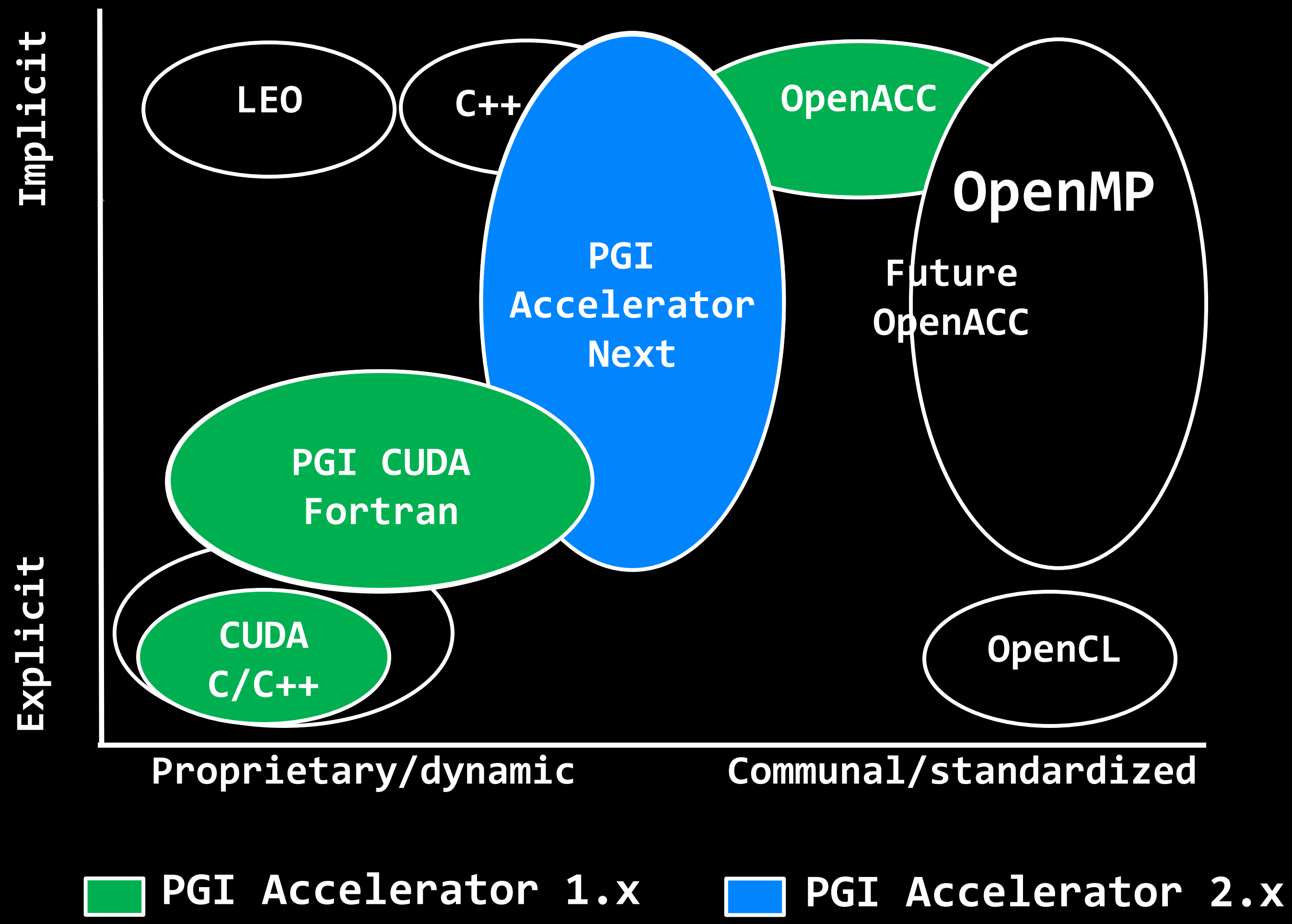
```
__kernel__ void mm_kernel(float *a, float *b,
           float *c, int n, int m, int l ) {
  float cij;
  int i, j, kg, k, wx, wy;
  __shared__ float asub[16][17], bsub[16][17];
  wx = workerIdx.x;
  wy = workerIdx.y;
  i = gangIdx.x * 16 + wx;
  j = gangIdx.y * 16 + wy;
  cij = 0.0f;

  for (kg = 0; kg < m; kg += 16) {
    asub[wy][wx] = a[(kg+wy)*n+i];
    bsub[wy][wx] = b[j*l+(kg+ty)];
    syncworkers();
    for (k = 0; k < 16; k++)
      cij += asub[k][wx] * bsub[wy][k];
    syncworkers();
  }
  c[j*n+i] = cij;
}
```

Host Code

Accelerator Code

Accelerator Language Landscape



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Object-oriented features

Type extension allows polymorphism:

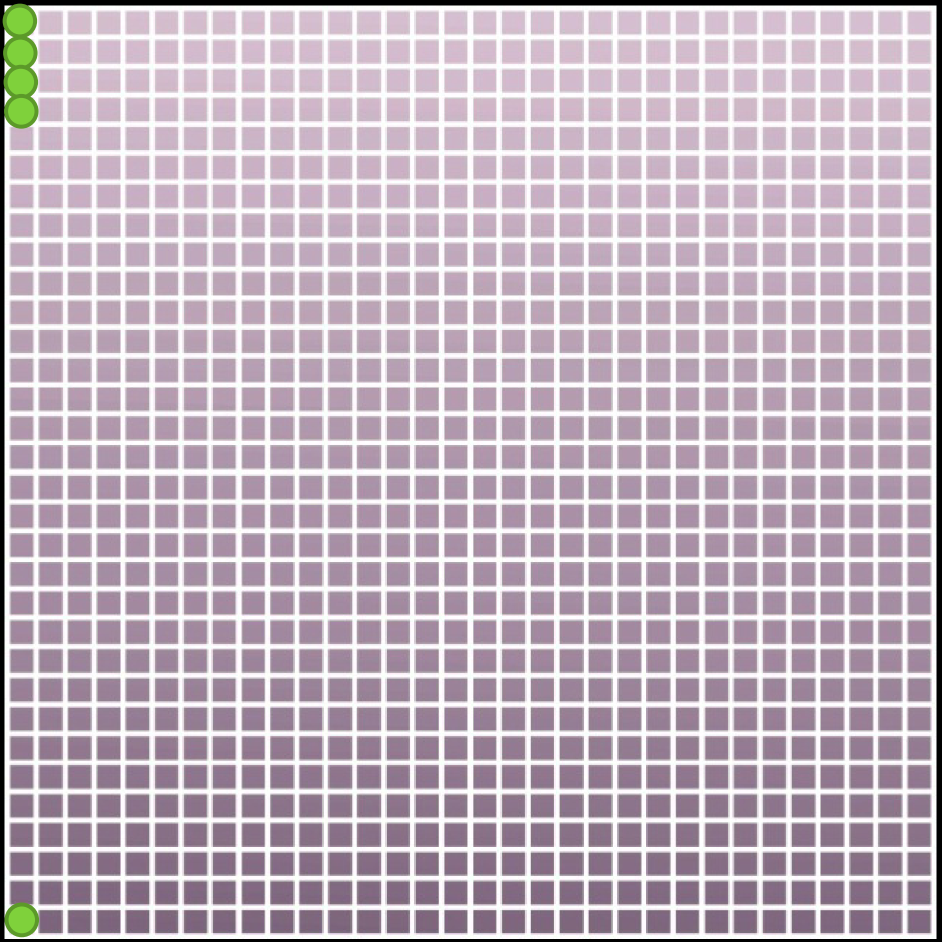
```
type dertype
integer  id, iop, npr
real, allocatable :: rx(:)
contains
  procedure :: init => init_dertype
  procedure :: print => print_dertype
  procedure :: find  => find_dertype
end type dertype

type, extends(dertype) :: extdertype
real, allocatable, device :: rx_d(:)
contains
  procedure :: init  => init_extdertype
  procedure :: find  => find_extdertype
end type extdertype
```

The class statement allows arguments of the base or extended type:

```
subroutine init_dertype(this, n)
class(dertype) :: this
```

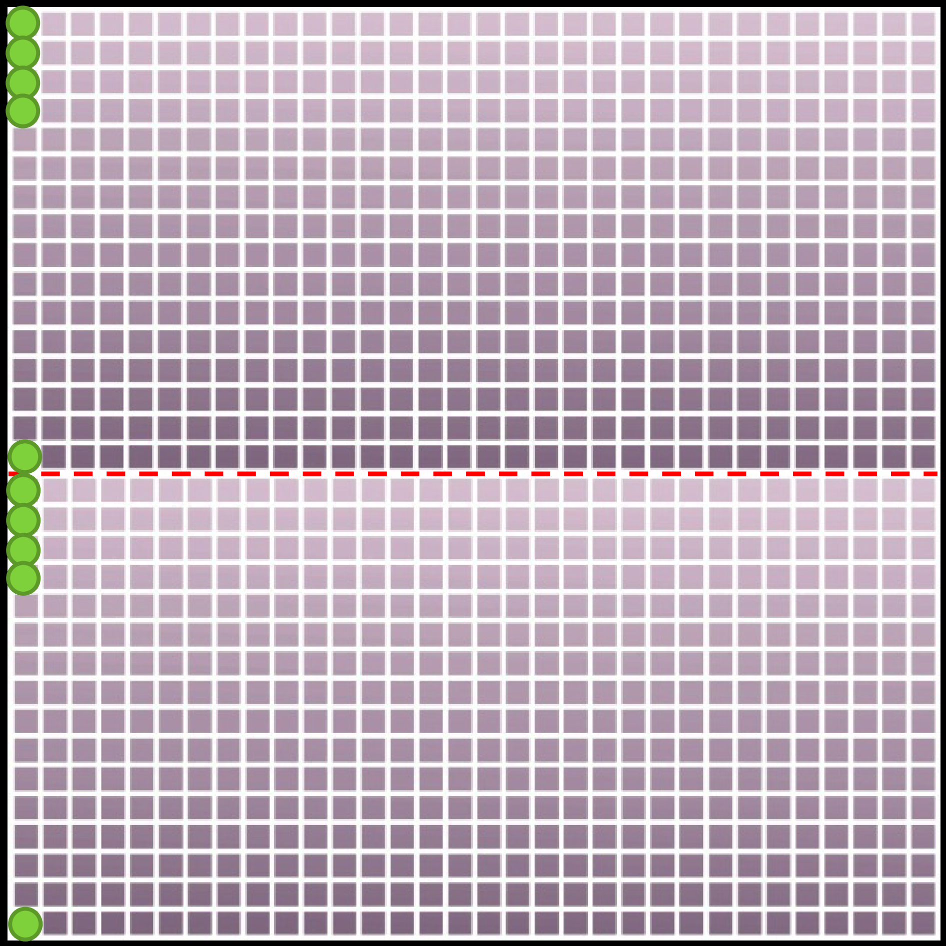
Single core scalar execution model

```
. . .
< statement >
< statement >

   for (i=0; i<N; i++) {
      for (j=0; j<M; j++) {
          f(i, j) ;
      }
   }

< statement >
. . .
```



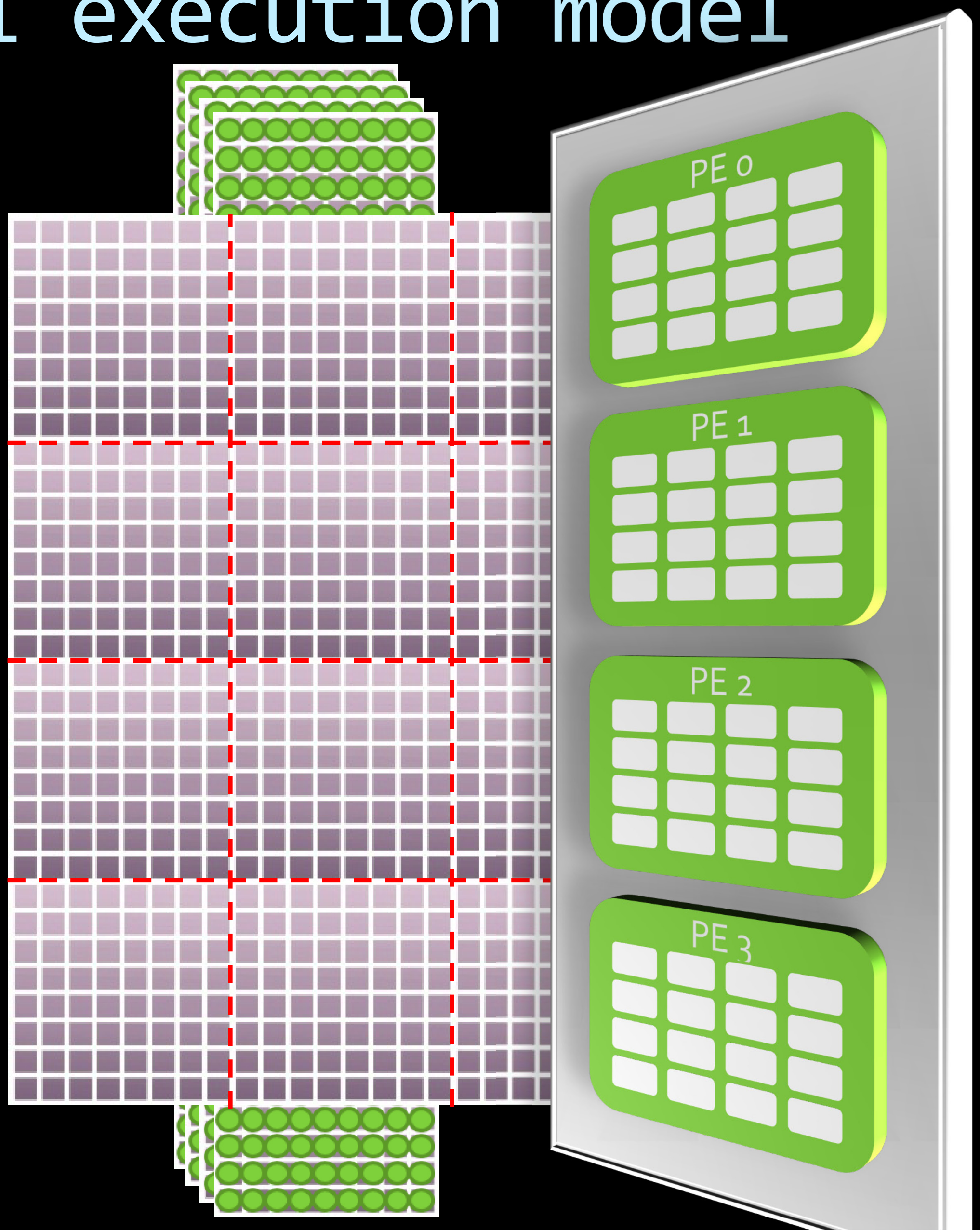
Dual core parallel execution model

```
. . .
< statement >
#pragma omp parallel
{
#pragma omp for
    for (i=0; i<N; i++) {
        for (j=0; j<M; j++) {
            f(i, j) ;
        }
    }
}
< statement >
. . .
```



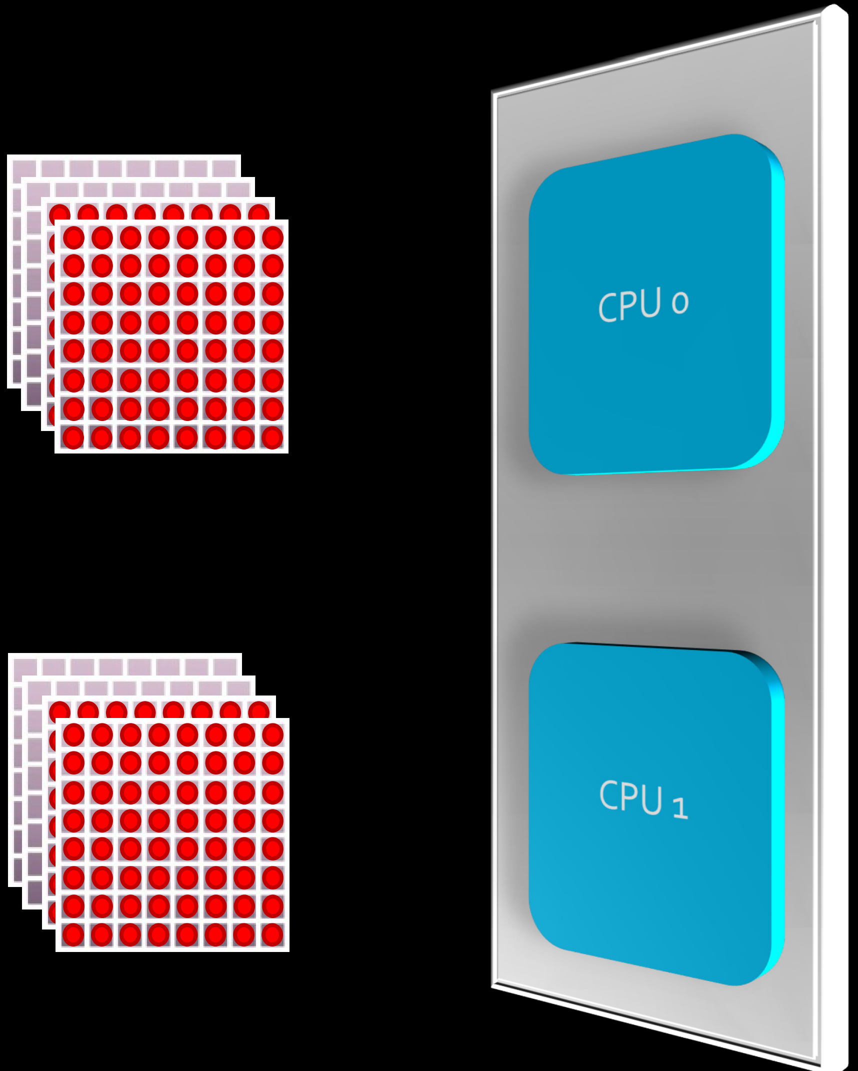
OpenCL kernel execution model

```
{
     int i ;
     int j ;

     i = get_global_id(0) ;
     j = get_global_id(1) ;
     f(i, j) ;
}
```

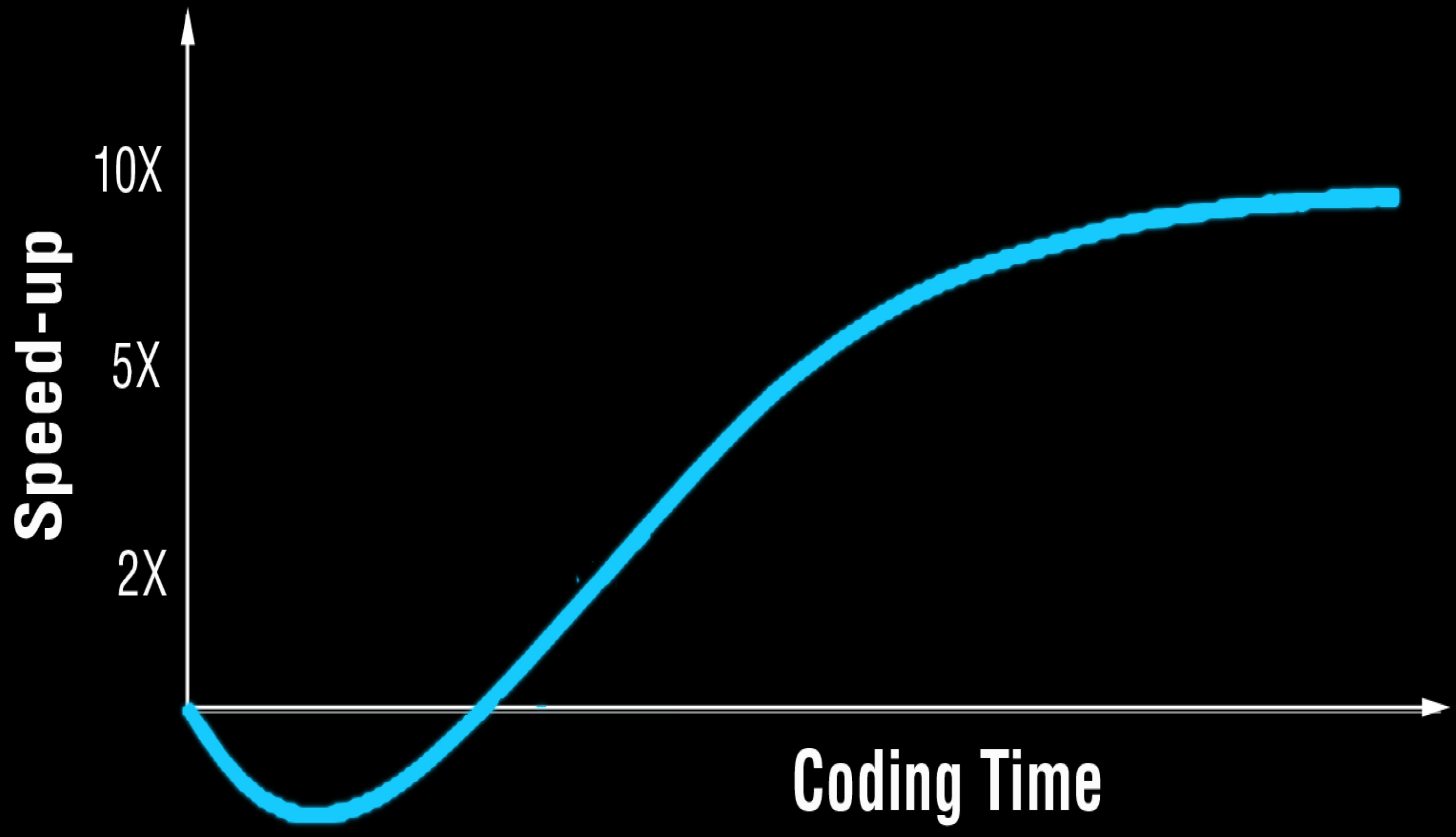


OpenCL kernel execution model on dual Cortex-A9

- Customizable Max WorkGroup size (256 Max)
- One pthread per CPU dedicated to manage WorkGroup execution
- 3 executions modes
  - Any WorkGroup size, no synchronization.
  - Any WorkGroup size, with synchronization. WorkItems are emulated by Light Weight Threads
  - WorkGroup size of 1 WorkItem with synchronization. Synchronization is 'nop-ified'

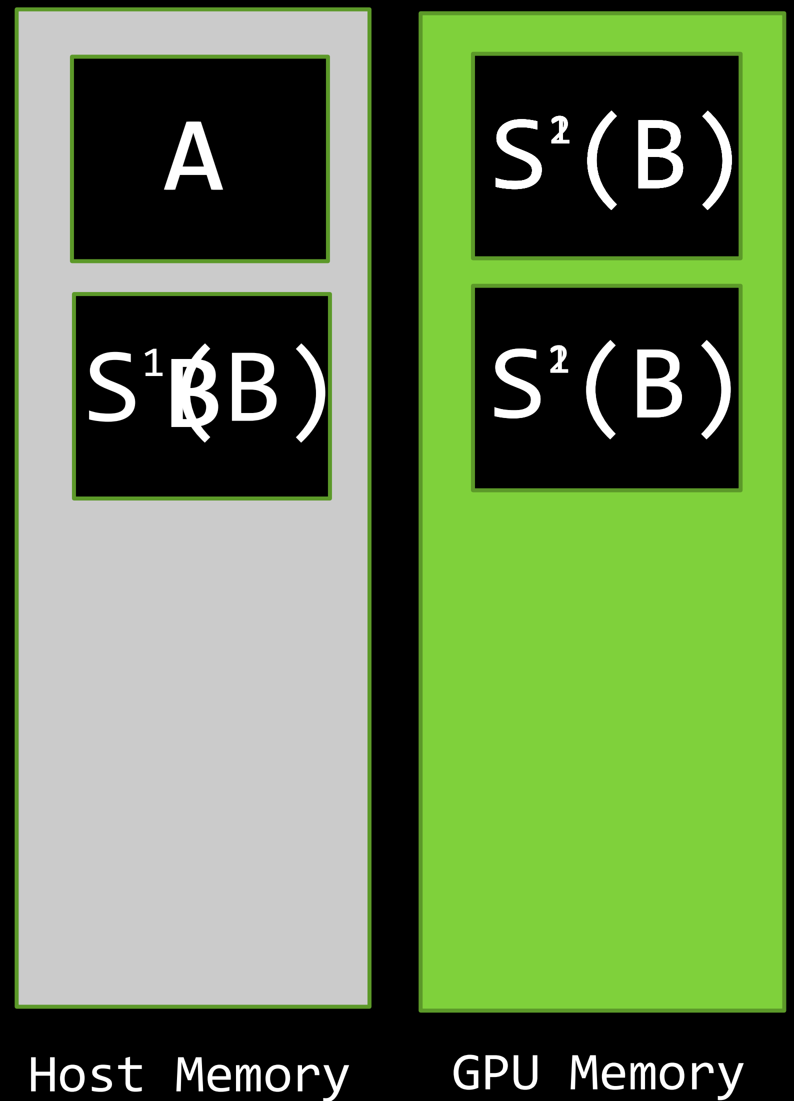


Typical Porting Experience with PGI Accelerator OpenACC Directives



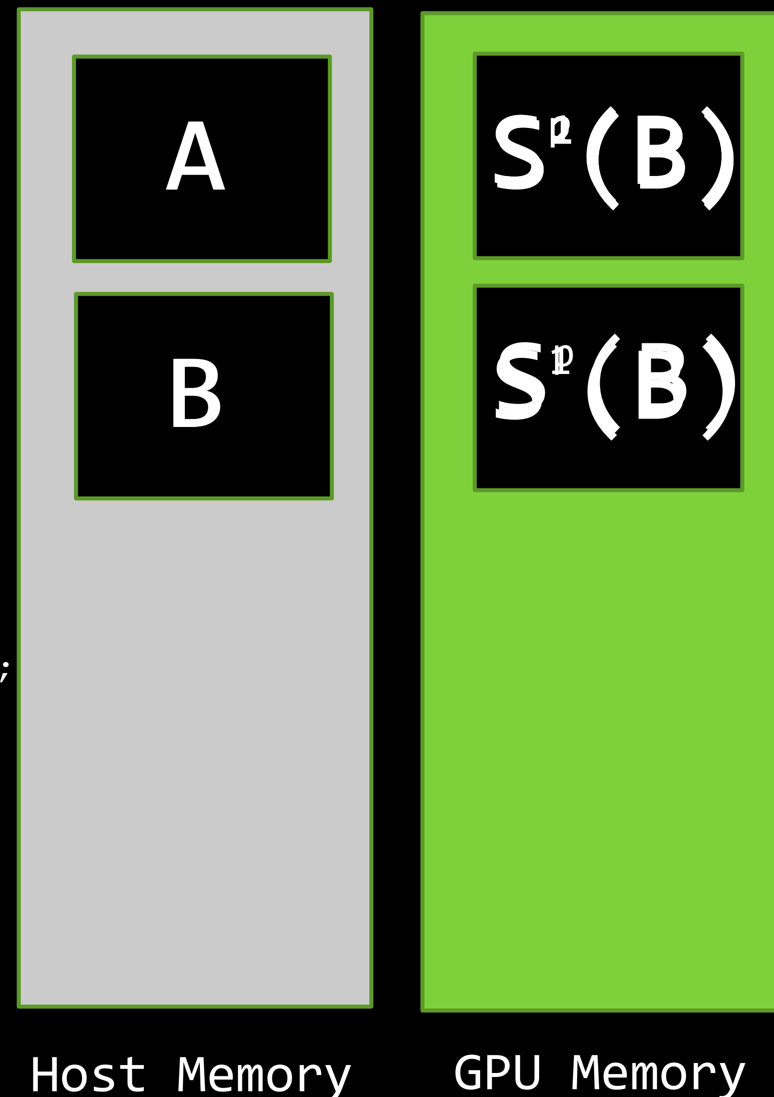
PGI Accelerator compute region

```
for (iter = 1; iter <= niters; ++iter){
  #pragma acc region
  {
  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];
  }
}
```



PGI Accelerator data region

```
#pragma acc data region \
        copy(b[0:n-1][0:m-1]) \
        local(a[0:n-1][0:m-1])
{
for (iter = 1; iter <= p; ++iter){
  #pragma acc region
  {
  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];
  }
}
}
```



OpenACC Abstract Machine Architecture