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**Bundesamt für Meteorologie und Klimatologie MeteoSchweiz**

# Accelerating climate models with GPUs using OpenACC

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# Goals of the training

- Provide an introduction on key aspects and challenges related to GPU computing

- Present minimal set of OpenACC directives to enable climate scientist to start porting a model to GPU / understand OpenACC directives in an existing code

# Content

- Introduction, GPU computing and directives
- Generating GPU kernels with OpenACC
- Data management with OpenACC
- Other OpenACC features
- Validation and performance

Material available at
**https://github.com/C2SM-RCM/OpenACC_Training**

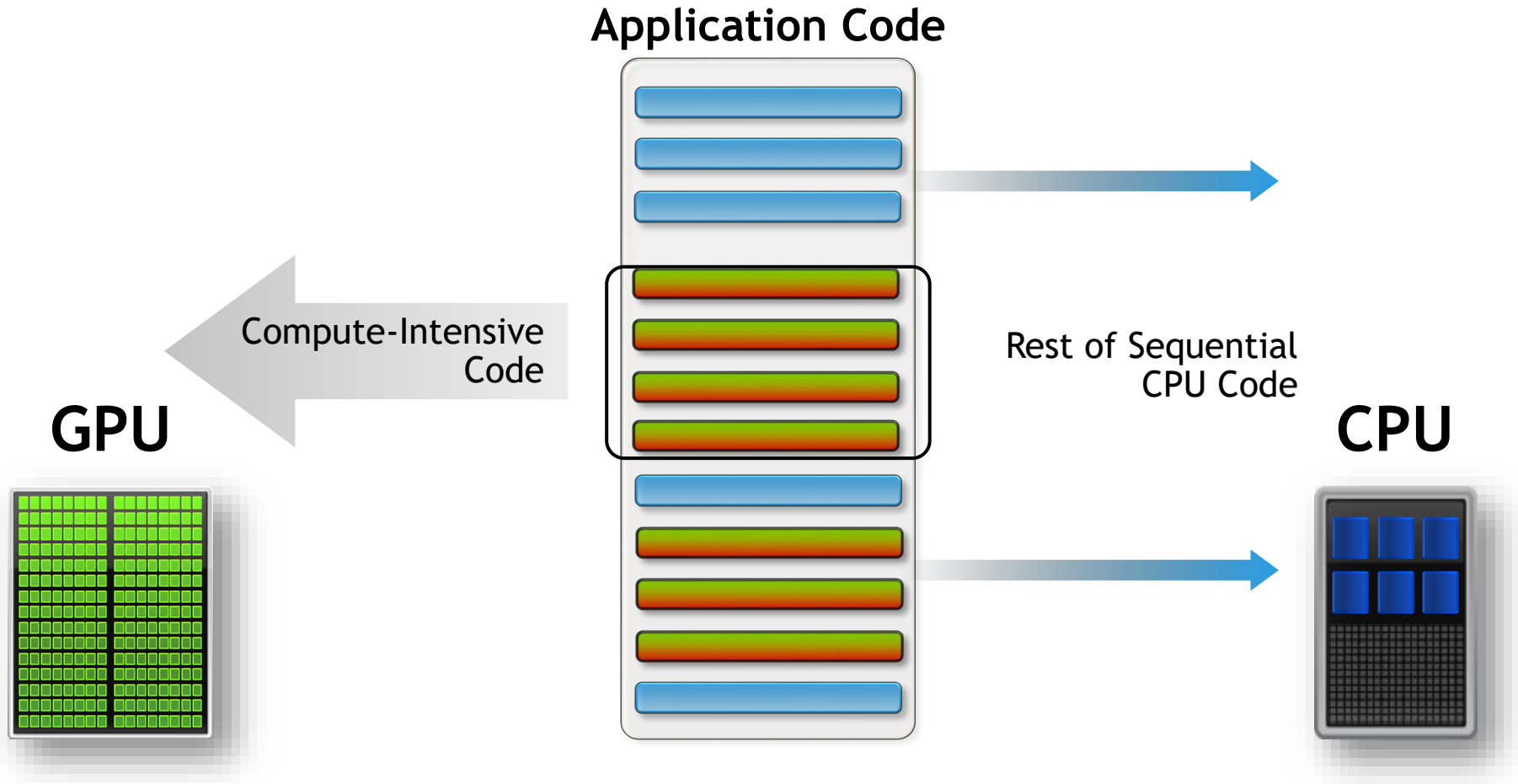
# Motivation: why using new hardware?

- They are already there!
- Most of the largest supercomputers are based on GPU accelerator
- Easier to get allocation time on GPU based system when effectively using the GPUs

What is GPU computing

- GPU = Graphical Processing Units
- GPU computing: use of a GPU to offload (intensive) parts of an application, while the remainder is computed on the CPU

# GPU computing: hybrid approach

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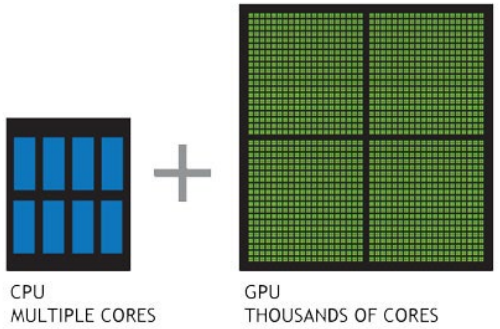
# GPU computing: key aspects

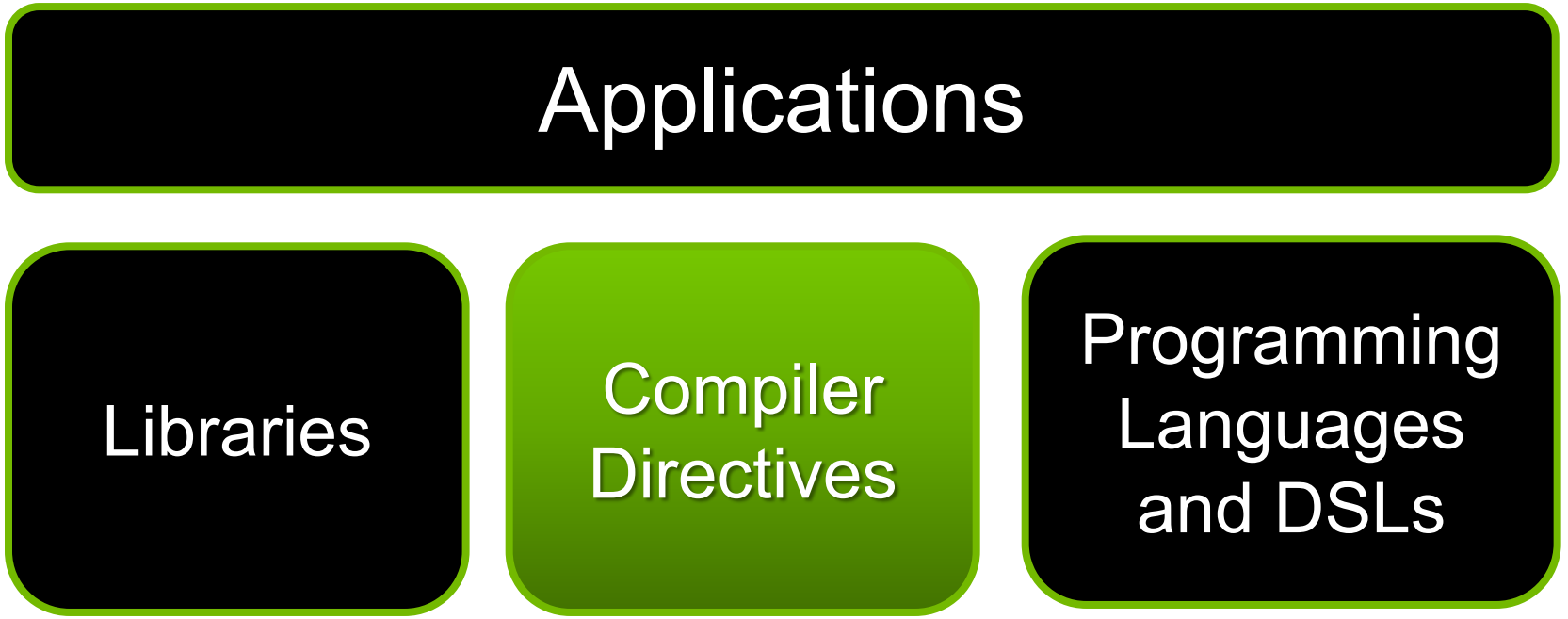
- GPUs have thousands of compute cores: need to express fine-grain parallelism




- GPU and CPU have (currently) separate physical memory
  - requires specific data management
  - data transfer may be a performance issue (slow transfer via PCI bus)

- As compared to typical multicore CPUs, GPUs have:
  - 5-10x higher peak performance (double precision)
  - 3-5x higher memory bandwidth

# 3 Ways to use GPUs

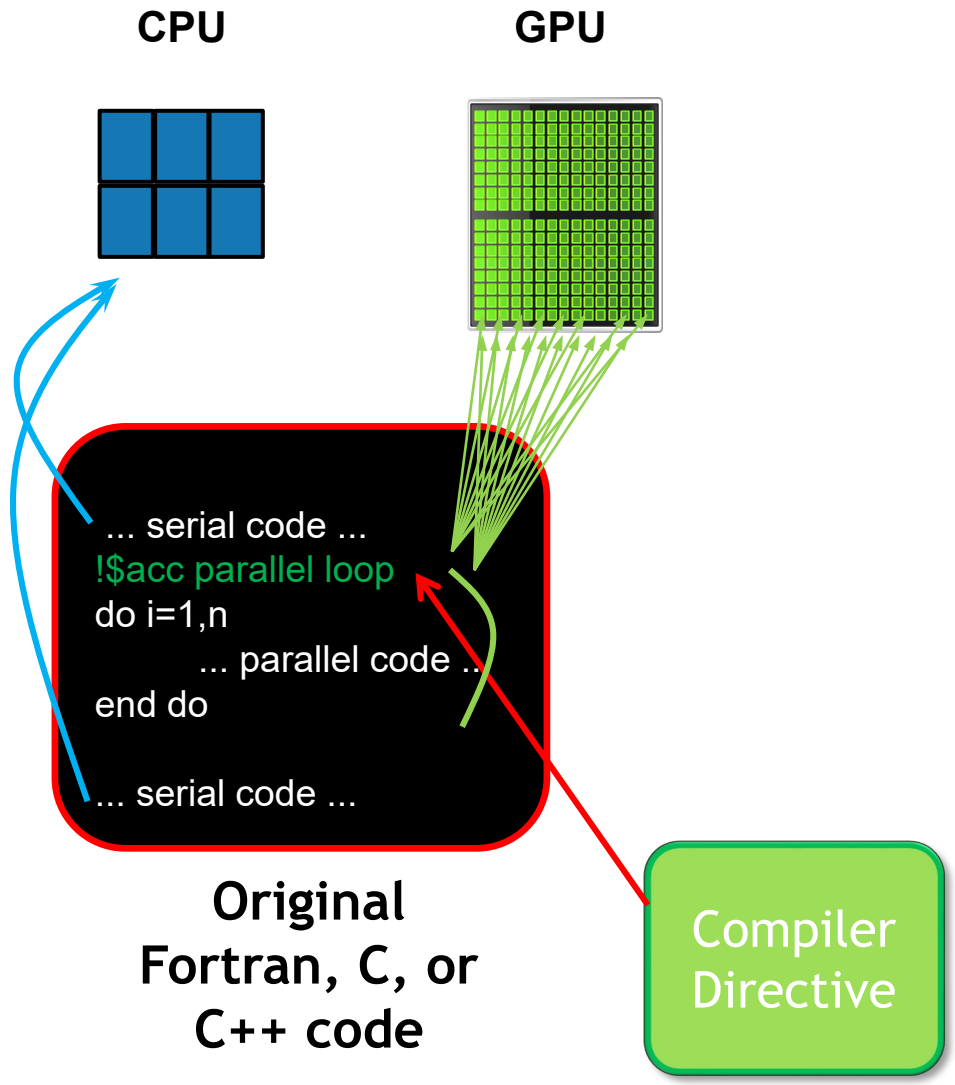



Ex: Magma, CULA, cuBLAS …

Ex: OpenACC, OpenMP

Cuda, Cuda Fortran, OpenCL, STELLA

# What are compiler directives?




- Compiler directives are comments or pragmas which can be inserted into existing code
- When a compiler directive is encountered the compiler/runtime will…

1. Generate parallel code for GPU
2. Allocate GPU memory and copy input data
3. Execute parallel code on GPU
4. Copy output data to CPU and deallocate GPU memory

- Directives are ignored on architecture without GPU

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# OpenACC

- OpenACC is a specification for high-level, compiler directives for expressing parallelism for accelerators in Fortran/C and C++.
  - Aims to be performance portable to a wide range of accelerators.
  - Multiple Vendors, Multiple Devices, One Specification
  - Nvidia GPU and AMD GPU (Cray only)
- The OpenACC specification was first released in November 2011.
  - Compilers: Cray, Nvhpc (nvidia), GCC
  - Latest official release Official web site: http://www.openacc.org

# OpenACC Directive Syntax

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

...often paired with a matching end directive surrounding a structured code block:

```
!$acc end directive
```

# Parallel and loop construct

**!$acc parallel** Starts parallel execution of the following section until the **!$acc end parallel**.

```
!$acc parallel
structured block
!$acc end parallel
```

**!$acc loop** [*clause*] applies to the immediately following loop, and describes the type of accelerator parallelism (vector, worker, gang) to use to execute the iterations of the loop. As a general rule all loop within a parallel region should have an !$acc loop

**!$acc loop seq** executes the loop sequentially

**!$acc loop** with no clause the compiler is free to choose the type of parallelism

# Example: SAXPY (y = a*x + y)

```
subroutine saxpy(n, a, x, y)
  real :: x(n), y(n), a
  integer :: n, i

  !$acc parallel
  !$acc loop
  do i=1,n
    y(i) = a*x(i)+y(i)
  enddo
  !$acc end parallel

end subroutine saxpy
```

This code region (kernel) will be executed in parallel on the GPU

Data management:

- Arrays x and y are automatically allocated and copied to the GPU
- y is automatically copied back to the CPU after the kernel execution
- scalars are automatically copied to the GPU

# What does “parallel” mean?

**Sequential (CPU)**

```
Load x(1)
Load y(1)
Compute a*x(1) + y(1)
Store y(1)
Load x(2)
Load y(2)
Compute a*x(2) + y(2)
Store y(2)
Load x(3)
Load y(3)
Compute a*x(3) + y(3)
Store y(3)
Load x(4)
Load y(4)
Compute a*x(4) + y(4)
Store y(4)
…
```

**Parallel (GPU)**

```
Load x(1), x(2), x(3), …
Load y(1), y(2), y(3), …
Compute a*x(:) + y(:)
Store y(1), y(2), y(3)
```

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# Toy model porting example

Available at:
**https://github.com/C2SM-RCM/OpenACC_Training/archive/master.zip**

Mimics the structure of a simplified atmospheric model having only physical parametrizations and output.

The code is structured as follows:

| | |
|---|---|
| main.f90 | main driver, calls init, time loop, and output |
| m_config.f90 | configuration information domain size, number of steps |
| m_fields.f90 | global fields |
| m_io.f90 | output routine |
| m_parametrization.f90 | physical parametrizations doing the actual computation |
| m_physics.f90 | driver for the physical paramtrization |
| m_setup.f90 | code initialization and clean up |
| m_timing.f90 | timing routines |

# Overview

main() in main.f90

```
CALL initialize()

!---------------------------------------
! time loop

WRITE(*,"(A)") "Start of time loop"

CALL start_timer(itimloop, "Time loop")

DO ntstep = 1, nstop

  ! call the physical parameterizations
  CALL physics()

  ! call outputs
  CALL write_output( ntstep )

END DO

CALL end_timer( itimloop )

WRITE(*,"(A)") "End of time loop"
```

physics() in:m_physics

```
! call a first physical parametrization
CALL saturation_adjustment(nx, ny, nz, t, qc, qv)

! call a second physical parametrization
CALL microphysics(nx, ny, nz, t, qc, qv)
```

saturation_adjustment(npx,npy,nlev,t,qc,qv) in m_parametrizations.f90

```
DO k = 1, nlev
  DO j = 1, npy
    DO i = 1, npx
      qv(i,j,k) = qv(i,j,k) + cs1*EXP(cs2*( t ...
      qc(i,j,k) = cs4*qv(i,j,k)
    END DO
  END DO
END DO
```

microphysics(npx,npy,nlev,t,qc,qv) in M_parametrizations.f90

```
DO k = 2, nlev
  DO j = 1, npy
    DO i = 1, npx
      qv(i, j, k) = qv(i,j,k-1) + cm1*  ...
      t(i, j, k)  = t(i, j, k)*( 1.0D0  ...
    END DO
  END DO
END DO
```

# Building and running OpenACC code on Daint

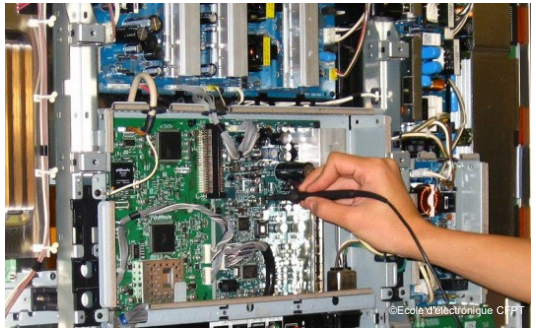
```
# log on daint via ela
ssh -Y login@ela.cscs.ch
ssh -Y daint.cscs.ch

# get code from ftp server
git clone git@github.com:C2SM-RCM/OpenACC_Training.git
cd OpenACC_Training

# setup environment
module load daint-gpu
module load PrgEnv-nvidia
module load craype-accel-nvidia60

cd handsOn
make TARGET=gpu COMPILER=nvidia handsOn1 # or TARGET=cpu
srun -n 1 -p debug -A d56 -C gpu ./handsOn1/handsOn1
```

# Hands-on 1




In directory handsOn1/

1. Compile and run handsOn without modification to get the CPU reference.
2. Save standard output in out_ref.txt.
3. Port subroutines param_a and param_b to GPU using the OpenACC parallel and loop constructs.
4. Run and check results against CPU.
5. How fast does your code run?
   Are you happy with the GPU acceleration?

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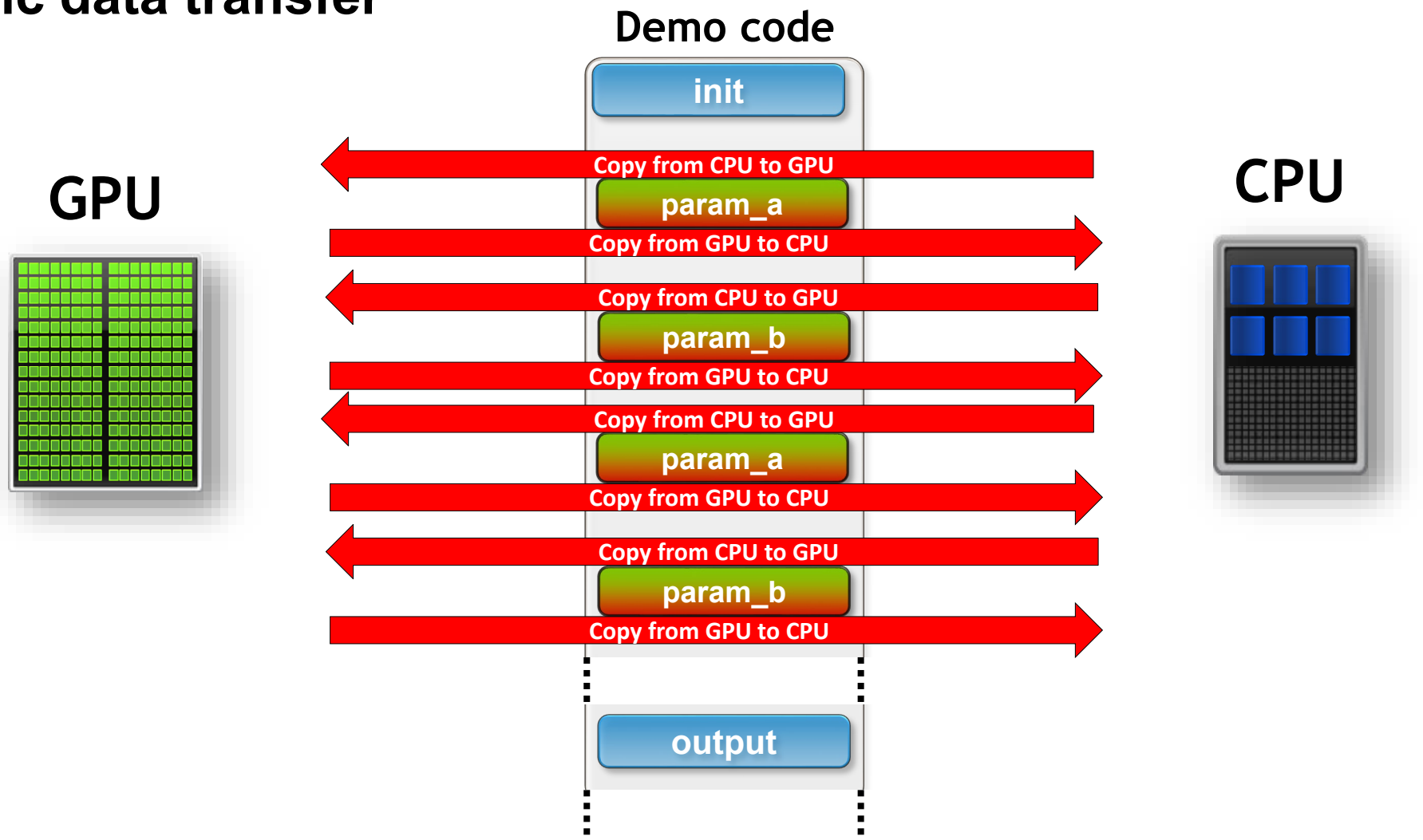
# Automatic data transfer



# Data constructs

In order to avoid excessive data movement between the CPU and the GPU the programmer can manually allocate and transfer data on the GPU. Data can than be kept on the GPU and reused between different kernels

**!$acc enter data create**(var) : allocates var on the gpu. Should be called after the allocation of var on the cpu

**!$acc exit data delete**(var) : deallocates var on the gpu. Should be called before the deallocation of var on the cpu

**!$acc update device**(var) : copies data from CPU to GPU

**!$acc update host**(var) : copies data from GPU to CPU

# Present clause

**!$acc data present** (var): tell the compiler that var is already allocated on the GPU.
Valid until matching **!$acc end data.**

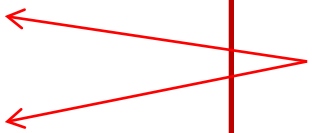
The compiler will not do any automatic data transfer for this variable between the **!$acc data present** and **!$acc end data** statements.

```
!$acc data present(var)
…
!$acc end data
```

# Example: SAXPY (y = a*x + y)

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

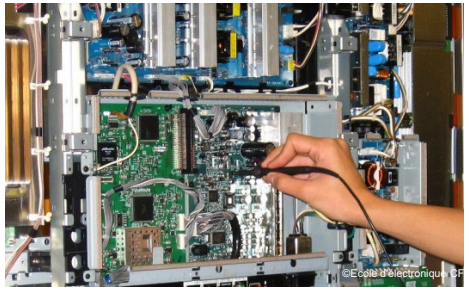
```
!allocate and copy to GPU
!$acc enter data create(arr1,arr2)
!$acc update device(arr1,arr2)

!first call to saxpy
call saxpy(n, a, arr1, arr2)

!second call to saxpy
call saxpy(n, a, arr1, arr2)

!copy back to CPU and deallocate GPU memory
!$acc update host(arr2)
!$acc exit data delete(arr1,arr2)
```



Data is kept on the GPU between the two calls to saxpy

Scalars are still automatically copied

# Hands-on 2



- Minimize data transfers using data constructs
- Keep initialization on the CPU
  1. Locate which array should be retain resident on the GPU.
  2. Allocate/deallocate on the GPU.
  3. Insert explicit data transfer.
  4. Avoid automatic copies for parallel regions.
  5. Check the *.lst files
  6. Check output against reference.
- How fast does your code run?
  How much time was spent in copying data?

# Part 2: explicit data placement 1/2

initialize() in m_setup.f90:

```
    ! print info
#ifdef _OPENACC
    WRITE(*,"(A)") "Running with OpenACC"
#else
    WRITE(*,"(A)") "Running without OpenACC"
#endif

    WRITE(*,"(A)") "Initialize"

    CALL init_timers()

    CALL start_timer( itiminit, "Initialization" )

    ! allocate memory
    ALLOCATE( t(nx,ny,nz), qv(nx,ny,nz) )

    ! allocate on the GPU
    !$acc enter data create(t,qv)

    ! initialize global fields
    DO k =1, nz
      DO j = 1, ny
        DO i = 1, nx
          t(i,j,k)  = 293.0D0 * (1.2D0 + 0.07D0 *
          qv(i,j,k) = 1.0D-6 * (1.1D0 + 0.13D0 * C
        END DO
      END DO
    END DO

    ! initialize fields on the GPU
    !$acc update device(t,qv)

#ifdef  OPENACC
```

Preprocessor macro defined when compiling with OpenACC

Allocation on GPU

Copy data from CPU to GPU

# Part 2: 2/2

saturation_adjustment

```
!$acc data present(t,qv,qc)
! do the computation
!$acc parallel
!$acc loop
DO k = 1, nlev
  !$acc loop
  DO j = 1, npy
    !$acc loop
    DO i = 1, npx
      qv(i,j,k) = qv(i,j,k) +
```

Present directive ensures no GPU-CPU transfer

microphysics:

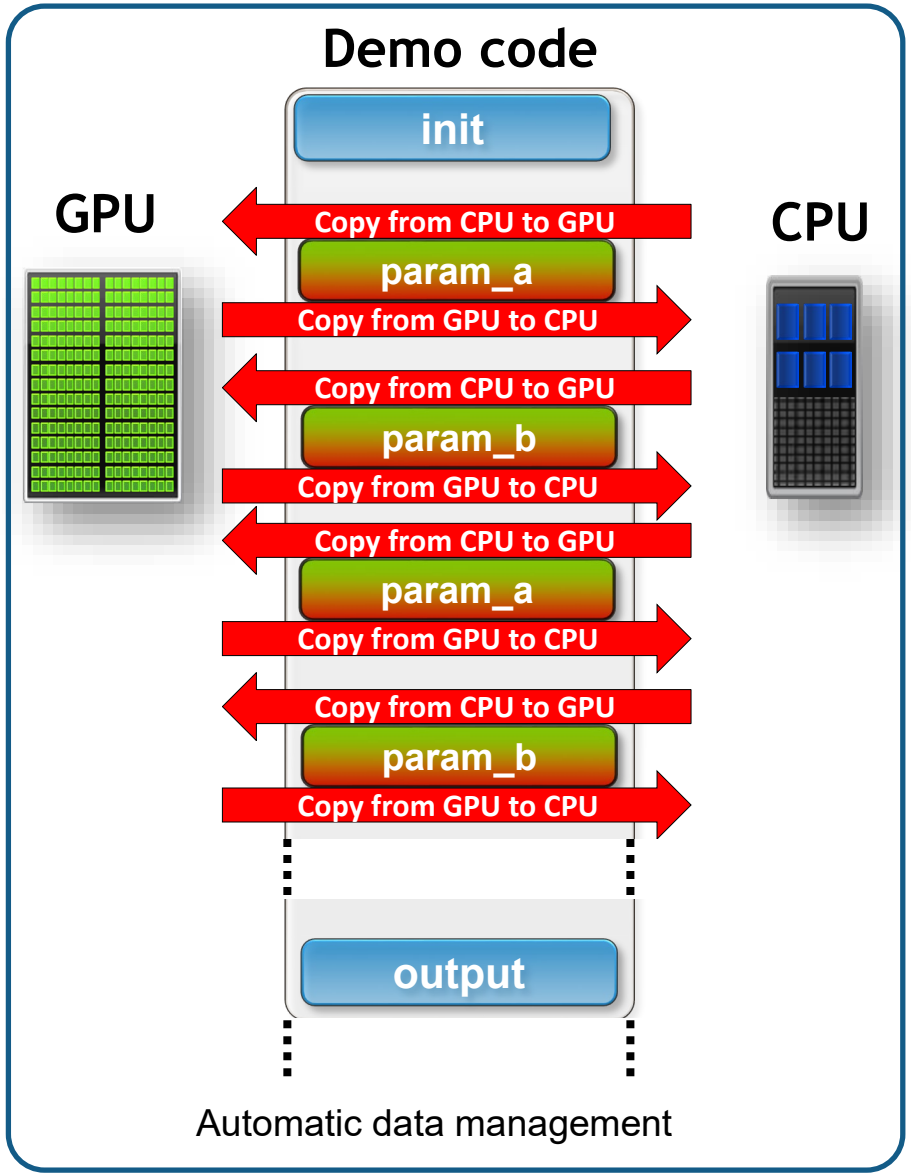
```
!$acc data present(t,qv,qc)
! do the computation
!$acc parallel
!$acc loop seq
DO k = 2, nlev
  !$acc loop
  DO j = 1, npy
    !$acc loop
    DO i = 1, npx
      qv(i, j, k) = qv(i,j,k-1) +
```

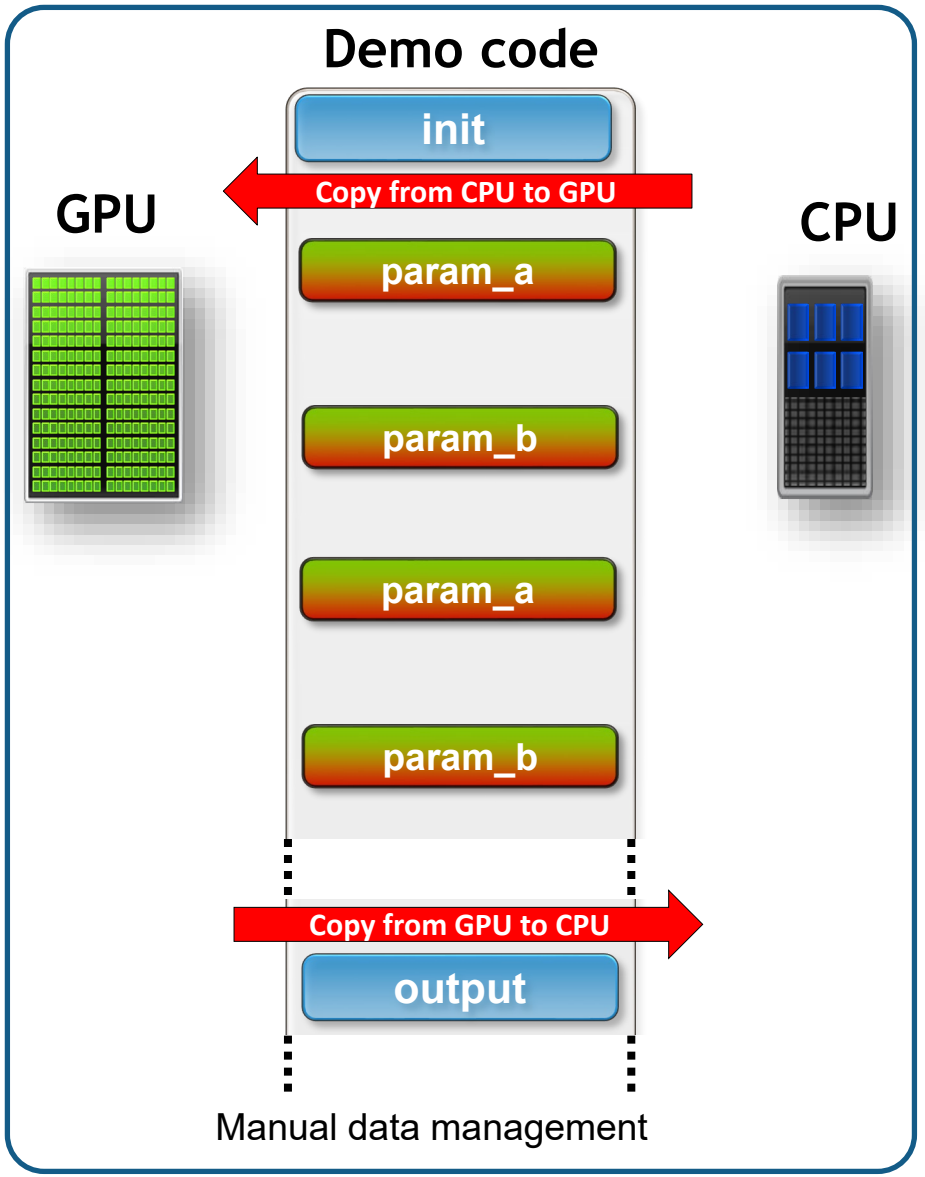
write_output() in m_io.f90

```
! skip if this is not a output timestep
IF (MOD(ntstep, nout) /= 0) RETURN
!$acc update host(qv)
```

Copy data from GPU to CPU only for output steps

# Automatic vs. manual data management



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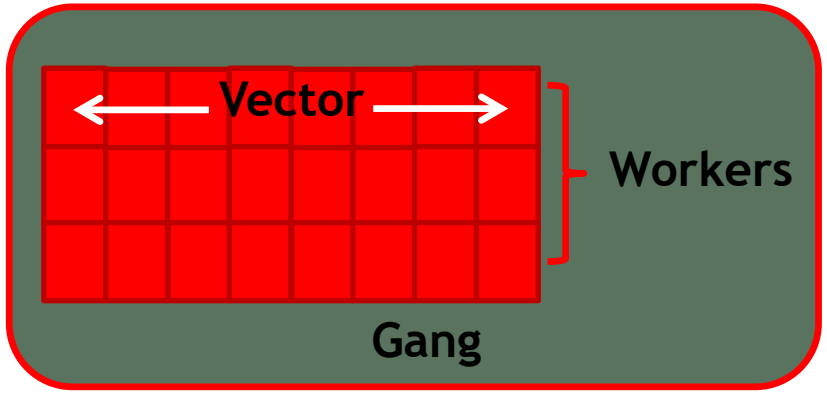
# OpenACC: 3 Levels of Parallelism

Additional keyword to address how parallelism is mapped to hardware:




- *Vector* threads work in lockstep (SIMD/SIMT parallelism)
- *Workers* have 1 or more vectors.
- *Gangs* have 1 or more workers and share resources (such as cache, the streaming multiprocessor, etc.)
- Multiple gangs work independently of each other

For best performance the *vector* parallelism should be associated with the stride one index loop. This corresponds to the left most index in Fortran.

# Example using gang, vector

```
subroutine saxpy2d(n, a, x, y)
  real :: x(n,n), y(n,n), a
  integer :: n, i
  !$acc parallel present(x,y)
  !$acc loop gang
  do j=1,n
   !$acc loop vector
   do i=1,n
    y(i,j) = a*x(i,j)+y(i,j)
   end
  enddo
  !$acc end parallel
end subroutine saxpy2d
```

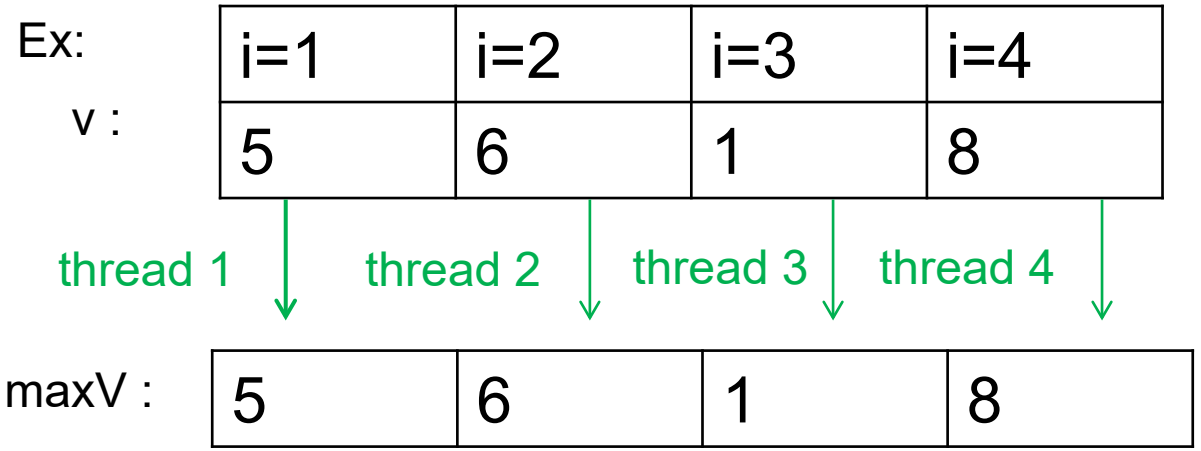
The **collapse** directive can be used to apply same parallelism to tightly nested loops

```
subroutine saxpy2d(n, a, x, y)
  real :: x(n,n), y(n,n), a
  integer :: n, i
  !$acc parallel present(x,y)
  !$acc loop gang vector collapse(2)
  do j=1,n
    do i=1,n
    y(i,j) = a*x(i,j)+y(i,j)
   end
  enddo
  !$acc end parallel
end subroutine saxpy2d
```

# Other OpenACC features: reduction

```
!assumes v >= 0
maxV=0
do i=1,n
  maxV=max(maxV,v(i))
end do
```

If i loop is run in parallel all threads will write in maxV => race condition.




maxV will have the value of the last thread writing at this location (i.e. any of 5,6,1,8)
=> Undefined behaviour, non reproducible.

# Reduction and atomic clause

**reduction**(op:var): At the end of the loop, the values for each thread are combined using the specified reduction operator, and the result stored in the original variable at the end of the parallel or kernels region. Note: should appear on each parallel loop

```
!assumes v >= 0
maxV=0
!$acc parallel present(v)
!$acc loop gang vector reduction(max:maxV)
do i=1,n
  maxV=max(maxV,v(i))
end do
!$acc end parallel
```

Valid Fortran operators are **+**, ***, max**, **min**, **iand**, **ior**, **ieor**, .**and.**, **.or.**, **.eqv.**, **.neqv.**

See also: **atomic** clause to prevent simultaneous access to a memory location

# OpenACC `Routine` Directive

The routine directive specifies that the compiler should generate a device copy of the function/subroutine in addition to the host copy.

Clauses:

```
!$acc routine [gang/worker/vector/seq]
```

# OpenACC Routine: Fortran

```
subroutine foo(v,i,j)
!$acc routine seq
  integer i,j
  real :: v

      v = 1.0/(i*j)

end subroutine

!$acc parallel
!$acc loop gang
do j=1,n
   !$acc loop vector
   do i=1,n
    call foo(v(i,j),i,i)
  endod
enddo
!$acc end parallel
```

The `routine` directive may appear in a fortran function or subroutine definition, or in an interface block.

Nested acc routines require the routine directive within each nested routine.

The save attribute is not supported.

# Private variables

- Scalar variables are by default first private over the gang not the thead
- This means that the same memory storage *could* be used by all vector threads.
- Scalars which need to be thread private (i.e. scalar on the left side of the "=" statement within the LOOP VECTOR) need to be made private on the vector loop.
- Scalar which are parameters for the considered kernel should be left with their default, i.e. no openACC statement. Note that loop variables are by default thread private and do not need a private statement.

```
!$ACC PARALLEL DEFAULT(NONE) ASYNC(1)
!$ACC LOOP SEQ
DO ic = 1, i_count
  jj = idx_lst(ic, jb)
  !$ACC LOOP GANG VECTOR PRIVATE(xx)
  DO jc = i_startidx, i_endidx
    xx = A(jc) ** 2.
    p_prog%B(jj, jb) = xx
  ENDDO
ENDDO
!$ACC END PARALLEL
```

# Derived type

- OpenACC supports derived types only since Version 2.6
- Derived types with allocatable or pointer components need special care
- pointer/allocatable vs. statically allocated array
  - Static components (scalar and fixed-size arrays) are copied with the derived types
  - Allocatable components have to be copied individually
- If the components are already on the device, they need to be attached explicitly to the derived type
- Update only individual components of a derived type
- An update directive applied on a derived type updates also the pointer references, which leads to invalid memory references

```
type :: t_container
  integer           :: scal
  real, allocatable :: allo(:)
  real, pointer     :: poin(:)
  real              :: stat(500)
end type t_container

type(t_container) :: con
[…]
allocate(con% allo(500), con% poin(500))
```

```
!$ACC ENTER DATA COPYIN(con)
!$ACC ENTER DATA COPYIN(con% allo, con% poin)
[…]
!$ACC EXIT DATA COPYOUT(con% allo, con% poin)
!$ACC EXIT DATA COPYOUT(con)
```

p_derived_type_0_enter_A.f90

```
!$ACC ENTER DATA COPYIN(con% allo, con% poin)
!$ACC ENTER DATA COPYIN(con)
!$ACC ENTER DATA ATTACH(con% allo, con% poin)
[…]
!$ACC EXIT DATA COPYOUT(con% allo, con% poin)
!$ACC EXIT DATA COPYOUT(con)
```

p_derived_type_0_enter_B.f90

Slide from Marek Jacob, DWD, Intro part 1

# Derived type

- Safest way is to create base derived type and components on device first and update needed components individually
- If a variable is already present on device a copy/copyin/copyout does not update device/self
- By updating individual components we can restrict memory transfer to those components, which are needed on device/sel
- The attach counter keeps track whether the pointers are attached or not

```
type :: t_container
  integer           :: scal
  real, allocatable :: allo(:)
  real, pointer     :: poin(:)
  real              :: stat(500)
end type t_container

type(t_container) :: con
[…]
allocate(con% allo(500), con% poin(500))
```

```
!$ACC ENTER DATA CREATE(con)
!$ACC ENTER DATA CREATE(con% allo, con% poin)

!$ACC UPDATE DEVICE(con% scal, con% allo)&
!$ACC   DEVICE(con% poin, con% stat)

[…]

!$ACC UPDATE SELF(con% scal, con% allo) &
!$ACC   SELF(con% poin, con% stat)

!$ACC EXIT DATA DELETE(con% allo, con% poin)
!$ACC EXIT DATA DELETE(con)
```

p_derived_type_0_enter_C.f90

Slide from Marek Jacob, DWD, Intro part 1

# Kernels vs parallel construct

- ACC KERNELS are similar to PARALLEL regions
- A kernels region gives the compiler maximum freedom of the parallel implementation
- Might be better or much worse than manual parallelization, may be compiler dependent
- Use of kernels is not recommended
- Implicit Fortran loops need to be replaced by explicit loops in a parallel region

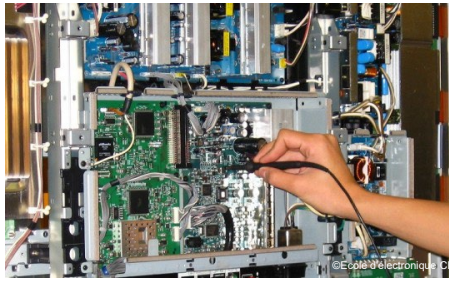
```
!$ACC KERNELS
do i = 1, n
  a(i) = 2.0 * b(i)
end do
!$ACC END KERNELS
```

```
!$ACC KERNELS
a(:) = 0.0
!$ACC END KERNELS

!$ACC PARALLEL LOOP
do i = 1, n
  a(i) = 0.0
end do
!$ACC END PARALLEL
```

Slide from Marek Jacob, DWD, Intro part 1

# Hands-on 3



- Add explicit gang and vector clause
- Try what happens when only adding gang clause on i-loop
- Compute output results (Sum a) on the GPU

```
sum_a=0
do k=1,nz
    do j=1,ny
      do i=1,nx
        sum_a=sum_a+a(i,j,k)
      end do
    end do
  end do
```

- Bonus: adapt physics to call saturation_adjustment and microhysics in the same i,j-loops, and use acc routine directive

# Content

- Introduction, GPU computing and directives
- Generating GPU kernels with OpenACC
- Data management with OpenACC
- Other OpenACC features
- Validation and performance

# Validation

- Both CPU and GPU implement IEEE-754 compliant floating point operations
  a+b or a*b will give the same results = bitwise identical

However:

- Transcendental functions are not defined, compiler dependent
- Compiler may (or not) use so called: fused add multipy

⇒ In general CPU and GPU results are not bitwise identical

Note: CPU codes compiled with two compilers are in general not bitwise identical

- Validations: requires to define acceptable thresholds, e.g. by perturbing reference CPU results to the last bit

# Perfomance


- Great care is required when evaluating performance, what is being compared . What is the expected performance?
- We often use socket to socket comparison, expectation based on hardware characteristic, compare **multicore** CPU vs GPU
- Use profiler, nsys, … : memory bandwidth, Flops …