OpenACC:
Productive, Portable Performance on Hybrid Systems Using High-Level Compilers and Tools

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(with contributions from Heidi Poxon)

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Piz Daint

Top500 List - November 2013

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
6	Swiss National Supercomputing Centre (CSCS) Switzerland	Piz Daint - Cray XC30, Xeon E5-2670 8C 2.600GHz, Aries interconnect , NVIDIA K20x Cray Inc.	115984	6271.0	7788.9	2325

The Green500 List

Listed below are the November 2013 The Green500's energy-efficient supercomputers ranked from 1 to 10.

Green500 Rank	MFLOPS/W	Site*	Computer*	Total Power (kW)
1	4,503.17	GSIC Center, Tokyo Institute of Technology	TSUBAME-KFC - LX 1U-4GPU/104Re-1G Cluster, Intel Xeon E5-2620v2 6C 2.100GHz, Infiniband FDR, NVIDIA K20x	27.78
2	3,631.86	Cambridge University	Wilkes - Dell T620 Cluster, Intel Xeon E5-2630v2 6C 2.600GHz, Infiniband FDR, NVIDIA K20	52.62
3	3,517.84	Center for Computational Sciences, University of Tsukuba	HA-PACS TCA - Cray 3623G4-SM Cluster, Intel Xeon E5-2680v2 10C 2.800GHz, Infiniband QDR, NVIDIA K20x	78.77
4	3,185.91	Swiss National Supercomputing Centre (CSCS)	Piz Daint - Cray XC30, Xeon E5-2670 8C 2.600GHz, Aries interconnect , NVIDIA K20x Level 3 measurement data available	1,753.66

OpenACC at SC13

Timetable

- 13:00 Introduction and accelerator primer (lecture)
- 13:20 A first introduction to OpenACC (lecture)
- 14:00 Porting a simple code (worked example)

- 14:30 ---------- Break ----------

- 15:00 Performance tuning with OpenACC (lecture)
- 15:30 Porting a more realistic code (worked example)
- 15:50 Asynchronicity and parallel applications (lecture)
- 16:15The future roadmap for OpenACC (lecture)

- 16:30 ---------- Close ----------

Contents

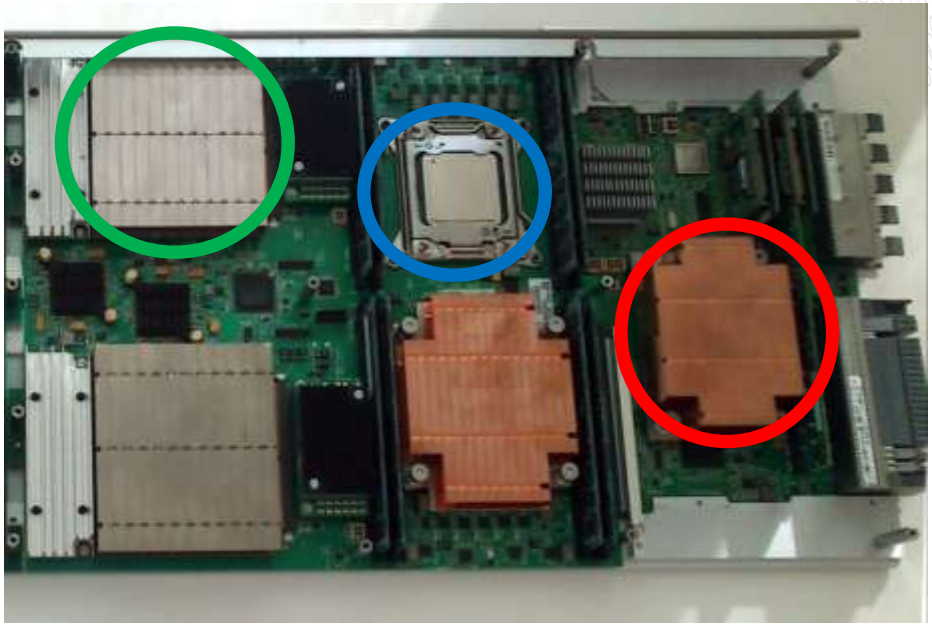
- **The aims of this course:**
  - To motivate why directive-based programming of GPUs is useful
  - To introduce you to the OpenACC programming model
  - To give you some experience in using OpenACC directives
    - with some hints and tips along the way
  - To introduce you to profiling tools
    - to understand and tune OpenACC performance
    - to help you understand a real application to start OpenACC-ing...
- **The idea is to equip you with the knowledge to develop applications that run efficiently on parallel hybrid supercomputers**
  - not just on single GPUs

Inside the Cray XC30 and the Nvidia Kepler K20X GPU

Alistair Hart
Cray Exascale Research Initiative Europe

The XC30 architecture

- **Node architecture:**
  - One Intel CPU
    - Sandybridge (8 cores)
    - Ivybridge (12 cores)
  - One Nvidia GPU
    - Kepler K20x or K40s
      - K20x: 2688 + 896 cores
        - 1.3 TFlop/s DP, 6GB memory



- **Cray Aries interconnect**
  - shared b/w 4 nodes on blade
  - Dragonfly network topology
    - 3 levels of all-to-all networks
  - high bandwidth/low latency scalability

- **Fully integrated/optimised/supported**
  - Tight integration of GPU and NIC drivers

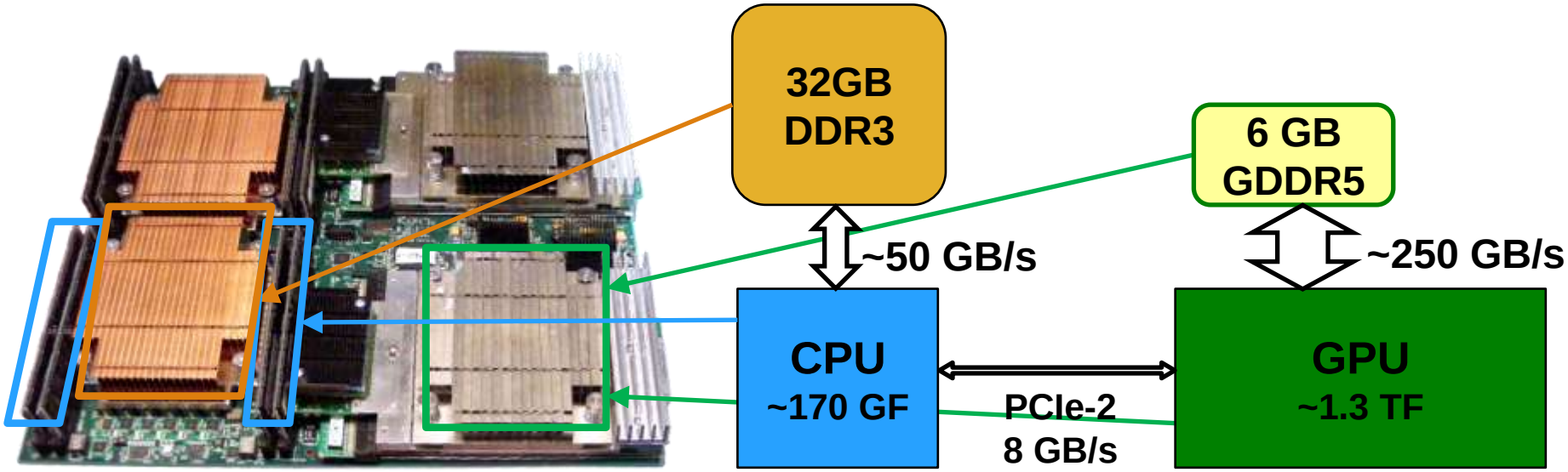
Exascale, but not exawatts

- **Power is a big consideration in an exascale architecture**
  - Jaguar XT (ORNL) drew 6MW to deliver 1PF
  - The US DoE wants 1EF, but using only 20MW...
- **A hybrid system is one way to reach this, e.g.**
  - 10^5 nodes (up from 10^4 for Jaguar)
  - 10^4 FPUs/node (up from 10 for Jaguar)
    - some full-featured cores for serial work
    - a lot more cutdown cores for parallel work
  - Instruction level parallelism will be needed
    - continues the SIMD trend SSE → AVX → ...
- **This looks a lot like the current GPU accelerator model**
  - manycore architecture, split into SIMT threadblocks
  - Complicated memory space/hierarchy (internal and PCIe)

A quick GPU refresher

How fast are current GPUs?

- **What should you expect?**
  - On a typical hybrid system (e.g. Cray XC30):
    - Flop/s: GPU ~8x faster than a single CPU (using all 8 cores)
    - Memory bandwidth: GPU ~5x faster than CPU
  - These ratios are going to be similar in other systems
- **Plus, it is harder to reach peak performance on a GPU**
  - Your code needs to fit the architecture
  - You also need to factor in data transfers between CPU and GPU

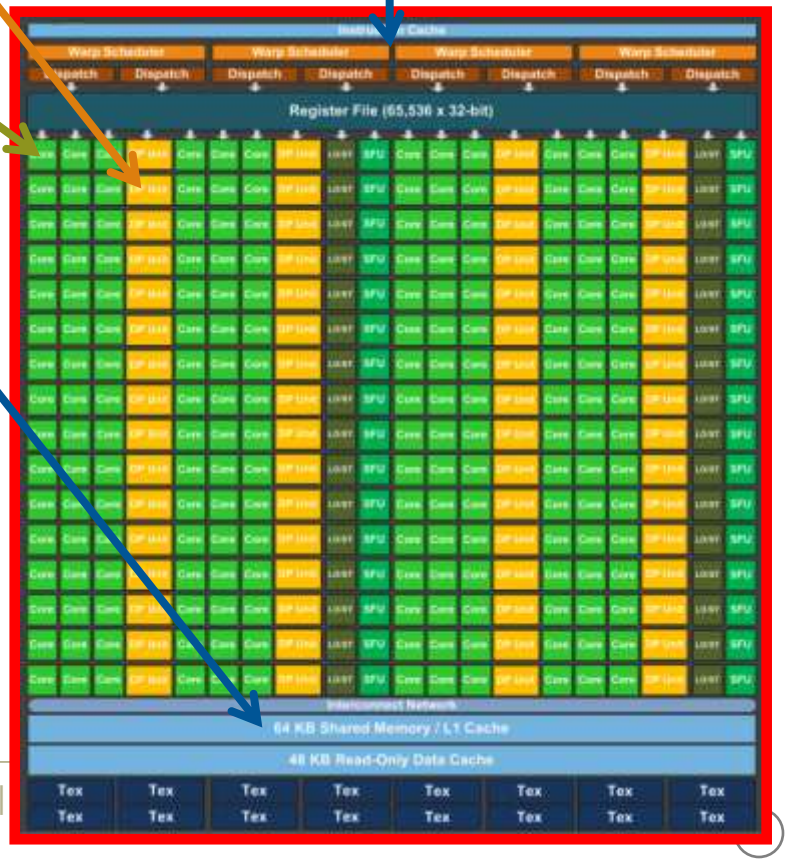


Nvidia K20X Kepler architecture (1)

- **Global architecture**
  - a lot of lightweight compute cores
    - 2688 SP plus 896 DP (ratio 3:1)
  - divided into 14 Streaming Multiprocessors (SMX)
  - SMXs operate independently of each other

Nvidia K20X Kepler architecture (2)

- **SMX architecture**
  - many cores (192 SP plus 64 DP)
  - shared instruction stream
    - lockstep, SIMT execution of same ops
    - SMX acts like vector processor
- **Memory hierarchy**
  - each core has private registers
    - fixed register file size
  - cores in an SM share a fast L1 cache
    - 64KB, split between:
      - L1 cache and user-managed
  - large global memory
    - shared by all SMXs (cores)
    - 6GB; also some specialist memory



Execution and memory models

- **Host-directed execution**
  - The main program executes on the host
    - The "host" can offload tasks to the "device" (accelerator, e.g. GPU)
      - tasks can be computation or data transfer between host and device
    - The host is responsible for managing the accelerator memory
      - as well as its own; allocating and freeing memory as needed
    - The host is responsible for synchronisation
      - ensuring offloaded tasks have completed

- **Weak memory model**
  - The host and device have separate memories
    - There's no automatic data synchronisation going on in the background
  - GPU memory is fragmented
    - there is no way to share data between all threads during computation
    - which leaves potential for race conditions

- **The compiler and runtime help much more with OpenACC**

Program execution with a GPU

- **The main program runs on the host (CPU)**
  - Some of the code will also execute on the host
    - either serially or in parallel with threads (e.g. OpenMP)
  - This code could be:
    - calculations that you want to be done on the CPU, e.g.
      - it is hard to parallelise for the GPU
      - there is not enough work to justify using the GPU
    - control statements for the GPU, e.g.
      - memory management
      - synchronisation
    - communication calls, e.g. MPI
- **The main program can also**
  - launch kernels (tasks) on the device (GPU)
  - These are written specially for the GPU, e.g. with
    - CUDA
    - OpenACC

Kernels

- **GPU kernels are executed by many threads in parallel**
  - all threads execute the same code
    - perform the same operations, but on different data
  - can take different paths in the code
    - actually, they all take the same paths but some threads spin
  - each thread has a unique ID
  - this can be used to
    - select which data elements to process
    - make control decisions
- **Threads are grouped together**
  - threads are grouped into "blocks" (or "gangs")
    - typically hundreds of threads per block
  - the group of blocks is called a "grid"

Kernel execution

- **Each kernel thread will be executed by a core on the GPU**
  - each threadblock will execute on a single SMX
    - you can have more threads than there are cores in an SMX
    - you really want this to happen
      - so the GPU has enough computational work
  - different threadblocks will execute on different SMXs
    - several threadblocks can be executing on the same SMX
    - you really want this to happen
      - threadblocks will be swapped in and out of execution to hide memory latency
    - you have no control over this
      - so you cannot predict which order threadblocks execute in
      - nor is there any way to impose a full barrier within a kernel
  - threads within a threadblock can interact
    - they can communicate data via a fast shared memory
    - you can synchronise within a threadblock

What CUDA doesn't tell you (upfront)

- **Threads are not created equal**
  - The SM is really a vector processor of width 32
    - groups of 32 cores act in lockstep, rather than independently
    - shares a single instruction stream with single program counter
    - Threads within a threadblock are divided into sets of 32 (warps)
    - each warp executes in SIMT fashion using 32 cores of SM
    - if a threadblock contains multiple warps, these are executed in turn
      - i.e. if there are more than 32 threads in the threadblock
  - Memory loads/stores are also done on a per-warp basis
    - Loading/storing 32 consecutive memory addresses at once
- **So, really, the compiler is implementing your code using vector instructions**
  - This is not explicit in the CUDA programming model, but is crucial to gaining good performance from a GPU
    - whichever programming model you are using (it's a hardware thing)

What does this mean for the programmer?

- You need a lot of parallel tasks (i.e. loop iterations) to keep GPU busy
  - Each parallel task maps to a thread in a threadblock
  - You need a lot of threadblocks per SM to hide memory latency
  - Not just 2688 parallel tasks, but 10^4 to 10^6 or more
  - This is most-likely in a loop-based code, treating iterations as tasks
    - OpenACC is particularly targeted at loop-based codes
- Your inner loop must vectorise (at least with vector length of 32)
  - So we can use all 32 threads in a warp with shared instruction stream
  - Branches in inner loop are allowed, but not too many
- Memory should be accessed in the correct order
  - Global memory access is done with (sequential) vector loads
  - For good performance, want as few of these as possible
  - so all the threads in warp should collectively load a contiguous block of memory at the same point in the instruction stream
  - This is known as "coalesced memory access"
  - So vectorised loop index should be fastest-moving index of each array

What does this mean for the programmer?

- No internal mechanism for synchronising between threadblocks
  - Synchronisation must be handled by the host
    - So reduction operations are more complicated
    - even though all threadblocks share same global memory
  - Fortunately launching kernels is cheap
    - GPU threadteams are "lightweight"

- Data transfers between CPU and GPU are very expensive
  - You need to concentrate on "data locality" and avoid "data sloshing"
  - Keeping data in the right place for as long as it is needed is crucial
  - You should port as much of the application as possible
    - This probably means porting more than you expected

OpenACC suitability

- **Will my code accelerate well with OpenACC?**
  - Computation should be based around loopnests processing arrays
    - Loopnests should have defined tripcounts (either at compile- or run-time)
      - while loops will not be easy to port with OpenACC
      - because they are hard to execute on a GPU
    - Data structures should be simple arrays
      - derived types, pointer arrays, linked lists etc. may stretch compiler capabilities
  - The loopnests should have a large total number of iterations
    - at least measured in the thousands
      - even more is better; less will execute, but with very poor efficiency
  - The loops should span as much code as possible
    - maybe with some loops very high up the callchain
  - The loopnest kernels should not be too branched
    - one or two nested IF-statements is fine
    - too many will lead to slow execution on many accelerators
  - The code can be task-based
    - but each task should contain a suitable loopnest

So...

- **GPUs can give very good performance**
  - but you need to be aware of the underlying architecture
  - porting a real application to GPU(s) requires some hard work
    - Amdahl says you need to port a lot of the profile to see a speed-up
      - bad news: to see 10x speedup, need to port at least 90% of the application profile
      - good news: if profile very peaked, 90% of time may be spent in, say, 40% of code
    - even before you worry about the costs of data transfers

- **A good programming model and environment**
  - helps bridges the gap between peak and achievable performance

Strategic risk factors of OpenACC

- **Will there be machines to run my OpenACC code on?**
  - Now? Lots of Nvidia GPU accelerated systems
    - Cray XC30s and XK7s, plus other vendors (OpenACC is multi-vendor)
  - Future? OpenACC can be targeted at other accelerators
    - PGI and CAPS already target Intel Xeon Phi, AMD GPUs
  - Plus you can always run on CPUs using same codebase

- **Will OpenACC continue?**
  - Support? Cray, PGI, CAPS committed to support. Now gcc as well.
    - Lots of big customer pressure to continue to run OpenACC
  - Develop? OpenACC committee now 18 partners
    - v2.0 finalised in 2013, now working on next version (2.1 or 3.0)

- **Will OpenACC be superseded by something else?**
  - Auto-accelerating compilers? Yes, please! But never managed before
    - Data locality adds to the challenge
  - OpenMP accelerator directives? Immature at the moment
    - OpenACC work not wasted: thinking takes more time than coding
    - Very similar programming model; can transition when these release if wish
    - Cray (co-chair), PGI very active in OpenMP accelerator subcommittee

Structure of this course

- **Aims to lead you through the entire development process**
  - What is OpenACC?
  - How do I use it in a simple code?
  - How do I port a real-sized application?
  - Performance tuning and advanced topics
- **It will assume you know**
  - A little bit about GPU architecture and programming
    - SMs, threadblocks, warps, coalescing
- **It will help if you know**
  - The basic idea behind OpenMP programming
    - but this is not essential

A first introduction to OpenACC

Contents

- **What is OpenACC?**
- **How do GPUs work?**
  - Will my code run well on a GPU using OpenACC?
- **What does OpenACC look like?**
- **How do I use it?**
  - The basic concepts
  - The basic directives
    - Advanced topics will have to wait for another training course
    - Like this one.

- **Plus a few hints, tips, tricks and gotchas along the way**
  - Not all guaranteed to be relevant, useful (or even true).

Accelerator programming

- **Why do we need a new GPU programming model?**
- **Aren't there enough ways to drive a GPU already?**
  - CUDA (incl. NVIDIA CUDA-C & PGI CUDA-Fortran)
  - OpenCL
- **All are quite low-level and closely coupled to the GPU**
  - User needs to rewrite kernels in specialist language:
    - Hard to write and debug
    - Hard to optimise for specific GPU
    - Hard to port to new accelerator
  - Multiple versions of kernels in codebase
    - Hard to add new functionality

Directive-based programming

Directives provide a high-level alternative

+ **Based on original source code (Fortran, C, C++)**
  + Easier to maintain/port/extend code
  + Users with OpenMP experience find it a familiar programming model
  + Compiler handles repetitive coding (cudaMalloc, cudaMemcpy...)
  + Compiler handles default scheduling; user tunes only where needed

– **Possible performance sacrifice**
  – Important to quantify this
  – Can then tune the compiler
  – Small performance sacrifice is an acceptable
    – trading-off portability and productivity against this
    – after all, who handcodes in assembler for CPUs these days?

OpenACC
Directives for Accelerators

CRAY

- **A common directive programming model for today's GPUs**
  - Announced at SC11 conference
  - Offers portability between compilers
    - Drawn up by: NVIDIA, Cray, PGI, CAPS
    - Multiple compilers offer:
      - portability, debugging, permanence
  - Works for Fortran, C, C++
    - Standard available at openacc.org
    - Initially implementations targeted at NVIDIA GPUs

- **Compiler support: all now complete**
  - Cray CCE: complete OpenACC 2.0 in v8.2
  - PGI Accelerator: v12.6 onwards
  - CAPS: Full support in v1.3
  - gcc:work started in late 2013, aiming for 4.9
  - Various other compilers in development

CAPS CRAY THE SUPERCOMPUTER COMPANY NVIDIA The Portland Group

Accelerator directives

- **Modify original source code with directives**
  - Non-executable statements (comments, pragmas)
    - Can be ignored by non-accelerating compiler
    - CCE -hnoacc also suppresses compilation
  - Sentinel: acc
    - C/C++: preceded by #pragma
      - Structured block {...} avoids need for end directives
    - Fortran: preceded by !$ (or c$ for FORTRAN77)
      - Usually paired with !$acc end * directive
      - Directives can be capitalized
  - Continuation to extra lines allowed
    - C/C++: \ (at end of line to be continued)
    - Fortran:
      - Fixed form: c$acc& or !$acc& on continuation line
      - Free form: & at end of line to be continued
        - continuation lines can start with either !$acc or !$acc&

```
// C/C++ example
#pragma acc *
{structured block}
```

```
! Fortran example
!$acc *
<structured block>
!$acc end *
```

Conditional compilation

- **In theory, OpenACC code should be identical to CPU**
  - only difference are the directives (i.e. comments)
- **In practise, you may need slightly different code**
  - For example, to cope with:
    - calls to OpenACC runtime API functions
    - where you need to recode for OpenACC
      - such as for performance reasons
      - you should try to minimise this
        - usually better OpenACC code is better CPU code
- **CPP macro defined to allow conditional compilation**
  - _OPENACC == yyyymm
    - Version 1.0: 201111
    - Version 2.0: 201306

A first example

- **Execute loop nest on GPU**

- **Compiler does the work:**
  - Data movement
    - determines data use in loopnest
    - at start and end of loopnest:
      - allocates/frees GPU memory
      - moves data to/from GPU
  - Synchronisation

```
#pragma acc parallel loop
for (j=0; j<N; j++) {
  for (i=1; i<N-1; i++) {
    c[j][i] = a[j][i] + b[j][i]
  }
}
```

write-only

read-only

  - Loop schedule: spreading loop iterations over threads of GPU
    - OpenACC will "partition" (workshare) more than one loop in a loopnest
      - compare this to OpenMP, which only partitions the outer loop

  - Caching (e.g. explicit use GPU shared memory for reused data)
    - automatic caching can be important

- User can tune all default behavior with optional clauses on directives

Accelerator kernels

- **We call a loopnest that will execute on the GPU a "kernel"**
  - this language is similar to CUDA
  - the loop iterations will be divided up and executed in parallel
- **We have choice of two directives to create a kernel**
  - parallel loop or kernels loop
    - both generate an accelerator computational task from a loopnest
      - also known as a "kernel"
      - the language is confusing
- **Why are there two and what's the difference?**
  - You can use either
    - or both, in different parts of the code
  - This tutorial concentrates on using the parallel loop directive

A first full OpenACC program: "Hello World"

```
PROGRAM main
  INTEGER :: a(N)
  <stuff>
!$acc parallel loop
  DO i = 1,N
   a(i) = i
  ENDDO
!$acc end parallel loop
!$acc parallel loop
  DO i = 1,N
   a(i) = 2*a(i)
  ENDDO
!$acc end parallel loop
  <stuff>
END PROGRAM main
```

- Two accelerator parallel regions
  - Compiler creates two kernels
    - Loop iterations automatically divided across GPU threads
  - First kernel initialises array
    - Compiler will determine a is write-only
  - Second kernel updates array
    - Compiler will determine a is read-write
  - Breaking parallel region=barrier
    - No barrier directive (global or within SM)

- Note:
  - Code can still be compiled for the CPU

Data scoping

- **Codes process data, using other data to do this**
  - all this data is held in structures, such as arrays or scalars

- **In a serial code (or pure MPI), there are no complications**
- **In a thread-parallel code (OpenACC, OpenMP etc.)**
  - Things are more complicated:
  - Some data will be the same for each thread (e.g. the main data array)
    - The threads can (and usually should) share a single copy of this data
  - Some data will be different (e.g. loop index values)
    - Each thread will need it's own private copy of this data

- **Data scoping arranges this. It is done:**
  - automatically (by the compiler) or explicitly (by the programmer)

- **If the data scoping is incorrect, we get:**
  - incorrect (and inconsistent) answers ("race conditions"), and/or
  - a memory footprint that is too large to run

Understanding data scoping

- **Data scoping ensures the right answer**
  - We want the same answer when executing in parallel as when serially

- **Declare variables in parallel region to be shared or private**
  - shared
    - all loop iterations process the same version of the variable
    - variable could be a scalar or an array
    - **a** and **b** are shared arrays in this example
  - private
    - each loop iteration uses the variable separately
    - again, variable could be a scalar or an array
    - **t** is a private scalar in this example
    - loop index variables (like **i**) are also private
  - firstprivate: a variation on private
    - each thread's copy set to initial value
    - loop limits (like **N**) should be firstprivate

```
for (i=0; i<N; i++) {
   t = a[i];
   t++;
   b[i] = 2*t;
}
```

Data scoping in OpenACC (and OpenMP)

- **In OpenMP, we have exactly these data clauses**
  - shared, private, firstprivate

- **In OpenACC**
  - private, firstprivate are just the same
  - shared variables are more complicated in OpenACC
    - because we also need to think about data movements to/from GPU
  - We sub-classify shared variables by how they are used on the GPU:
  - copyin: a shared variable that is used read-only by the GPU
  - copyout: a shared variable that is used write-only
  - copy: a shared variable that is used read-write
  - create: a shared variable that is a temporary scratch space (although there is still an unused copy on the host in this case)

Data scoping with OpenACC

- **parallel regions:**
  - scalars and loop index variables are private by default
  - arrays are shared by default
    - the compiler chooses which shared-type: copyin, copyout, etc.
  - explicit data clauses over-ride automatic scoping decisions

  - You can also add the default(none) clause
    - then you have to do everything explicitly (or you get a compiler error)

A more-explicit first version

```
PROGRAM main
  INTEGER :: a(N)
  <stuff>
!$acc parallel loop copyout(a)
  DO i = 1,N
   a(i) = i
  ENDDO
!$acc end parallel loop
!$acc parallel loop copy(a)
  DO i = 1,N
   a(i) = 2*a(i)
  ENDDO
!$acc end parallel loop
  <stuff>
END PROGRAM main
```

- **We could choose to make the data movements explicit**
  - maybe because we want to
    - maybe also use default(none) clause
  - or maybe compiler is overcautious

- Note:
  - Array a is needlessly moved from/to GPU between kernels
    - You could call this "data sloshing"
    - This will have a big impact on performance

OpenACC data regions

- **Data regions allow data to remain on the accelerator**
  - e.g. for processing by multiple accelerator kernels
  - specified arrays only move at start/end of data region
- **Data regions are only label a region of code**
  - they do not define or start any sort of parallel execution
  - just specify GPU memory allocation and data transfers
  - can contain host code, nested data regions and/or device kernels
- **Be careful:**
  - Inside data region we have two copies of each of the specified arrays
  - These only synchronise at the start/end of the data region
    - and only following the directions of the explicit data clauses
  - Otherwise, you have two separate arrays in two separate memory spaces

Defining OpenACC data regions

- **Two ways to define data regions:**
  - Structured data regions:
    - Fortran: !$acc data [data-clauses] ... !$acc end data
    - C/C++: #pragma acc data [date-clauses] {...}
  - Unstructured data regions (new in OpenACC v2):
    - Fortran: !$acc enter data [data-clauses] ... !$acc exit data [data-clauses]
    - C/C++: #pragma enter data [data-clauses] ... #pragma exit data [data-clauses]

- **For most "procedural code", use structured data regions**

- **Unstructured data regions**
  - Useful for more "Object Oriented" coding styles, e.g.
    - Separate constructor/destructor methods in C++
    - Separate subroutines for malloc (or allocate) and free (or deallocate)

- **A data region with no data clauses is pointless**
  - that is, it is redundant (and does nothing)

A second version

```
PROGRAM main
  INTEGER :: a(N)
  <stuff>
!$acc data copyout(a)
!$acc parallel loop
  DO i = 1,N
   a(i) = i
  ENDDO
!$acc end parallel loop
!$acc parallel loop
  DO i = 1,N
   a(i) = 2*a(i)
  ENDDO
!$acc end parallel loop
!$acc end data
  <stuff>
END PROGRAM main
```

- Now added a data region
  - Specified arrays only moved at boundaries of data region
  - Unspecified arrays moved by each kernel
  - No compiler-determined movements for data regions
- Data region can contain host code and accelerator regions
- Copies of arrays independent

- **No automatic synchronisation within data region**
  - User-directed synchronisation possible with update directive

Data scoping with OpenACC (2)

- **parallel regions:**
  - scalars and loop index variables are private by default
  - arrays are shared by default
    - the compiler chooses which shared-type: copyin, copyout, etc.
  - explicit data clauses over-ride automatic scoping decisions
    - You can also add the default(none) clause
    - then you have to do everything explicitly (or you get a compiler error)

- **data regions:**
  - only shared-type scoping clauses are allowed
  - there is NO default/automatic scoping
  - un-scoped variables on data regions
    - will be scoped at each of the enclosed parallel regions
      - automatically, unless the programmer does this explicitly
    - this probably leads to unwanted data-sloshing or large arrays
  - Using data region scoping in enclosed parallel regions:
    - same routine: omit scoping clauses on enclosed parallel directives
    - different routine: use present clause on enclosed parallel directives

Sharing GPU data between subprograms

```
PROGRAM main
  INTEGER :: a(N)
  <stuff>
!$acc data copyout(a)
!$acc parallel loop
  DO i = 1,N
   a(i) = i
  ENDDO
!$acc end parallel loop
  CALL double_array(a)
!$acc end data
  <stuff>
END PROGRAM main
```

```
SUBROUTINE double_array(b)
  INTEGER :: b(N)
!$acc parallel loop present(b)
  DO i = 1,N
   b(i) = double_scalar(b(i))
  ENDDO
!$acc end parallel loop
END SUBROUTINE double_array
```

```
INTEGER FUNCTION double_scalar(c)
  INTEGER :: c
  double_scalar = 2*c
END FUNCTION double_scalar
```

- **present clause uses GPU version of b without data copy**
  - Original calltree structure of program can be preserved
- **One kernel is now in subroutine (maybe in separate file)**
  - OpenACC 1.0: function calls inside parallel regions required inlining
  - OpenACC 2.0: compilers support nested parallelism

Reduction variables

- **Reduction variables are a special case of private variables**
  - where we will need to combine values across loop iterations
  - e.g. sum, max, min, logical-and etc. acting on a shared array

- **We need to tell the compiler to treat this appropriately**
  - Use the reduction clause for this (added to parallel loop directive)
    - same expression in OpenACC as in OpenMP
  - Examples:
    - sum: use clause reduction(+:t)
      - Note sum could involve adding and/or subtracting
    - max: use clause reduction(max:u)

```
DO i = 1,N
   t = t + a(i) - b(i)
   u = MAX(u,a(i))
ENDDO
```

- **Note: OpenACC only allows reductions of scalars**
  - not of array elements
  - advice:
    - try rewriting to use a temporary scalar in the loopnest for the reduction

Data scoping gotchas: OpenACC vs. OpenMP

- **In OpenACC parallel regions:**
  - scalars *and* loop index variables are private by default
- **Compare this to OpenMP parallel regions:**
  - loop index variables are private by default, but scalars are shared
- **Be careful of this, especially:**
  - if you program (separately) using the two programming models, or
  - if you are translating an OpenMP code to OpenACC

Minimising data movements

- **This is the single-biggest OpenACC optimisation for GPUs**

- **There are three techniques:**
  - Keep data on the GPU as long as possible
    - use data regions and port all enclosed loopnests (as we have seen)
  - Only move arrays when you need to
    - using the update directive
  - Only move the data you need to move
    - using array sections

The update directive

- **Data regions keep data on device**
  - can span multiple compute kernels and serial (host) code
  - create *copies* of data arrays on device for duration of data region
  - host, device copies only synchronised at start/end of data region
    - as requested by explicit data clauses
- **You can synchronise copies manually within a data region**
  - for instance:
    - to copy a halo buffer back to the host for communication
    - to copy values of an array to the CPU for checking or printing
- **You do this using the update directive, for instance:**
  - update host(a) copies entire array a from device to host
    - OpenACC 2.0: can use self instead of host
  - update device(a) copies entire array a from host to device

Array sections

- **Sometimes we only need to move part of an array**
  - array section notation allows this, using ":" notation
  - syntax differs slightly between languages
    - Fortran uses start:end, so first N elements is a(1:N)
    - C/C++ uses start:length, so first N elements is b[0:N]
    - Advice: be careful when switching languages!
      - Use profiler, CRAY_ACC_DEBUG commentary to see how much data moved

- **Sections allowed in data clauses and with update**

- **For multi-dimensional arrays**
  - specified sections must be a contiguous block of memory
  - can only specify one incomplete section on slowest-moving index
    - Fortran: slowest index is right-most
      - so a(1:N,2:N-1) is allowed, but a(2:N-1,1:N) is not
    - C/C++: slowest index is left-most
      - so b[1:N-2][0:N] is allowed, but b[0:N][1:N-2] is not

Unshaped pointers

- **"Unshaped pointer" compiler/runtime errors**
  - Fortran arrays have a complicated data structure
    - includes a descriptor that contains information about size and shape
    - the compiler therefore knows how much data to transfer
  - C/C++: arrays are often just pointers
    - especially if the arrays were dynamically allocated or passed by reference
    - How many bytes should be transferred here: copy(c) ?
    - So you usually need to be more explicit
      - You need to put in data clauses
      - And specify the slicing (even if this is the whole array): copy(c[0:N])

Sharing data between kernels

- **If you are using a data region around kernels**
  - Must ensure that the runtime uses the shared data already present
- **If the kernel is in the same routine as the data region**
  - just don't mention those bits of data in the parallel/kernels clauses
- **If the kernel is in a different routine to the data region**
  - On the parallel or kernels directive:
    - Specify the relevant data with present clause
    - instead of other shared clauses (copy, copyin, copyout, create)
    - don't rely on automatic scoping for shared data in this case
- **If an array is declared present, but is not on accelerator**
  - you get a runtime error and the program crashes
  - This is usually what you would like to happen
    - rather than running to completion with the wrong answer
  - But there are other ways to do things...

Directives in summary

- **Compute regions**
  - created using parallel loop or kernels loop directives
- **Data regions**
  - created using data or enter/exit data directives
- **Data clauses are applied to:**
  - accelerated loopnests: parallel and kernels directives
    - here they over-ride relevant parts of the automatic compiler analysis
    - you can switch off all automatic scoping with default(none) clause (in v2)
  - data regions: data directive (plus enter/exit data in OpenACC v2)
    - There is no automatic scoping in data regions (arrays or scalars)
  - Shared clauses (copy, copyin, copyout, create)
    - supply list of scalars, arrays (or array sections)
  - Private clauses (private, firstprivate, reduction)
    - only apply to accelerated loopnests (parallel and kernels directives)
  - present clause (used for nested data/compute regions)

And take a breath...

- **You now know everything you need to start accelerating**
  - You can successfully port a lot of codes just knowing this much
  - The performance at this stage isn't bad, either
    - you can often beat the CPU version of the code running across all the cores
- **So what is the rest of OpenACC for?**
  - Some codes require more functionality to port
  - OpenACC also has a lot of performance tuning options
- **The emphasis in this introduction has been on**
  - explaining data scoping and using data regions
- **Why?**
  - because optimising data movements is far more important than tuning
    - minimising data transfers typically speeds up GPU execution by 10x-100x
    - performance tuning maybe gains you 2x-3x
      - and you can't start to get this until you first stop data-sloshing

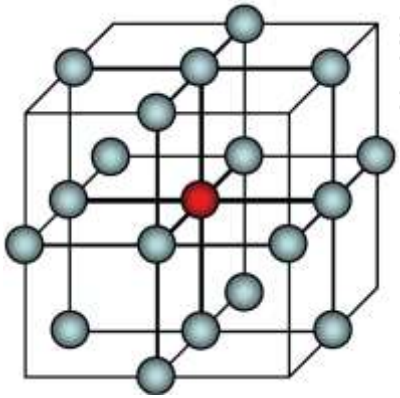
#pragma acc exit data

Do you have any questions?

Porting a Simple Code

Worked example: scalar Himeno code

The Himeno Benchmark



- **3D Poisson equation solver**
  - Iterative loop evaluating 19-point stencil
  - Memory intensive, memory bandwidth bound
- **Fortran and C implementations are available from** http://accc.riken.jp/2444.htm
- **We look here at the scalar version for simplicity**
  - We will discuss the parallel version later today
- **Code characteristics**
  - Around 230 lines of Fortran or C
  - Arrays statically allocated
    - problem size fixed at compile time

Why use such a simple code?

- **Understanding a code structure is crucial if we are to *successfully* OpenACC an application**
  - i.e. one that runs faster node-for-node
  - not just full accelerator vs. single CPU core

- **There are two key things to understand about the code:**
  - How is data passed through the calltree?
  - Where are the hotspots?

- **Answering these questions for a large application is hard**
  - There are tools to help
    - we will discuss some of them later in the tutorial
  - With a simple code, we can do all of this just by code inspection

The key questions in detail

- **How is data passed through the calltree?**
  - CPUs and accelerators have separate memory spaces
  - The PCIe link between them is relatively slow
  - Unnecessary data transfers will wipe out any performance gains
  - A successful OpenACC port will keep data resident on the accelerator
- **Where are the hotspots?**
  - The OpenACC programming model is aimed at loop-based codes
    - Which loopnests dominate the runtime?
    - Are they suitable for an accelerator?
      - What are the min/average/max tripcounts?
- **Minimising data movements will probably require acceleration of many more (and possibly all) loopnests**
  - Not just the hotspots
    - any loopnest that processes arrays that we want accelerator-resident
  - But we have to start somewhere

First stages to accelerating an application

1. **Understand and characterise the application**
   - Profiling tools, code inspection, speaking to developers if you can
2. **Introduce first OpenACC kernels**
3. **Introduce data regions in subprograms**
   - reduce unnecessary data movements
   - will probably require more OpenACC kernels

Next stages to accelerating an application

4. **Move up the calltree, adding higher-level data regions**
   - ideally, port entire application so data arrays live entirely on the GPU
   - otherwise, minimise traffic between CPU and GPU
   - This will give the single biggest performance gain

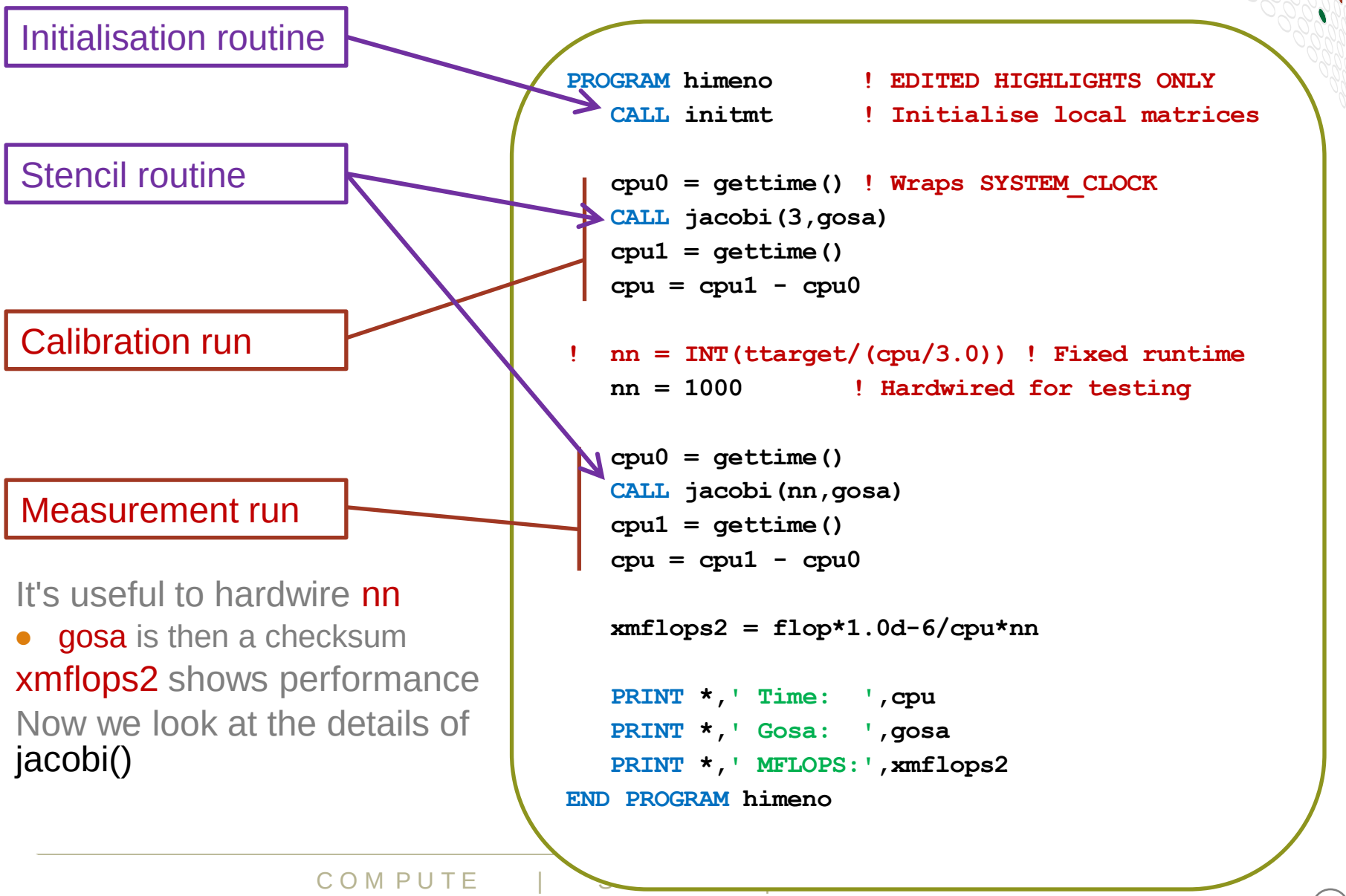
5. **Only now think about performance tuning for kernels**
   - First correct any obviously inefficient scheduling on the GPU
     - This will give some good performance improvements
   - Optionally, experiment with OpenACC tuning clauses
     - You may gain some final additional performance from this

- **And remember Amdahl's law...**

Run the initial CPU version of the code

- **First we compile and run the code "as is"**
  - on the CPU, using one core
  - compiled with Cray Compilation Environment (CCE)
- **The output reports:**
  - The runtime
    - `Measurement: Time (secs) :  4.804376120446249`8
  - The performance (from the runtime, in MFLOPS)
    - `Measurement: MFLOPS      :  2853.7552548501367`
  - A residual value from the solver (checksum)
    - `Measurement:  Gosa       : 0.13797154081596327E-02`

Step 1: Himeno program structure



- It's useful to hardwire nn
  - gosa is then a checksum
- xmflops2 shows performance
- Now we look at the details of jacobi()

Step 1: Structure of the jacobi routine

- **Iteration loop**
  - must be sequential!
- **Apply stencil to `p`**
  - create temporary **`wrk2`**
  - residual **`gosa`** computed
- **Update array `p`**
  - from **`wrk2`**
  - can be parallelised
  - outer halo unchanged

```
SUBROUTINE jacobi(nn,gosa)

  iter_lp: DO loop = 1,nn

! compute stencil: wrk2, gosa from p
     <described on next slide>

! copy back wrk2 into p
       DO k = 2,kmax-1
          DO j = 2,jmax-1
             DO i = 2,imax-1
                p(i,j,k) = wrk2(i,j,k)
             ENDDO
          ENDDO
       ENDDO

    ENDDO iter_lp

END SUBROUTINE jacobi
```

Step 1: The Jacobi computational kernel

- Stencil applied to array **p**
  - 19-point finite difference
- Not in-place:
  - Updated values saved in temporary array **wrk2**
- Residual value **gosa**
  - computed here
  - is a reduction variable
- This loopnest dominates runtime
  - Can be parallelised

```
gosa = 0d0
DO k = 2,kmax-1
 DO j = 2,jmax-1
  DO i = 2,imax-1
   S0=a(i,j,k,1)*p(i+1,j, k ) &
     +a(i,j,k,2)*p(i, j+1,k ) &
     +a(i,j,k,3)*p(i, j, k+1) &
     +b(i,j,k,1)*(p(i+1,j+1,k )-p(i+1,j-1,k ) &
                 -p(i-1,j+1,k )+p(i-1,j-1,k )) &
     +b(i,j,k,2)*(p(i, j+1,k+1)-p(i, j-1,k+1) &
                 -p(i, j+1,k-1)+p(i, j-1,k-1)) &
     +b(i,j,k,3)*(p(i+1,j, k+1)-p(i-1,j, k+1) &
                 -p(i+1,j, k-1)+p(i-1,j, k-1)) &
     +c(i,j,k,1)*p(i-1,j, k ) &
     +c(i,j,k,2)*p(i, j-1,k ) &
     +c(i,j,k,3)*p(i, j, k-1) &
     + wrk1(i,j,k)

   ss = (s0*a(i,j,k,4)-p(i,j,k)) * bnd(i,j,k)
   gosa = gosa + ss*ss
   wrk2(i,j,k) = p(i,j,k) + omega*ss
  ENDDO
 ENDDO
ENDDO
```

fwd n.n.
n.n.n.
bwd n.n.

Step 2: a first OpenACC kernel

- Start with most expensive
  - apply parallel loop
  - end parallel loop optional
    - *advice: use it for clarity*
- reduction clause
  - as in OpenMP, not optional
- private clause?
  - By default:
    - loop variables private
      - i, j, k
      - like OpenMP
    - scalar variables private
      - s0,ss
      - ***unlike*** OpenMP
  - so clause is optional here
  - Note that private arrays
    - always need private clause

```
gosa = 0d0

!$acc parallel loop reduction(+:gosa)

DO k = 2,kmax-1
 DO j = 2,jmax-1
  DO i = 2,imax-1
   s0 = a(i,j,k,1) * p(i+1,j, k ) &
     <etc...>

   ss = (s0*a(i,j,k,4) - p(i,j,k)) * &
                                 bnd(i,j,k)
   gosa = gosa + ss*ss
   wrk2(i,j,k) = p(i,j,k) + omega*ss
  ENDDO
 ENDDO
ENDDO
!$acc end parallel loop
```

Step 2: a first OpenACC kernel (contd)

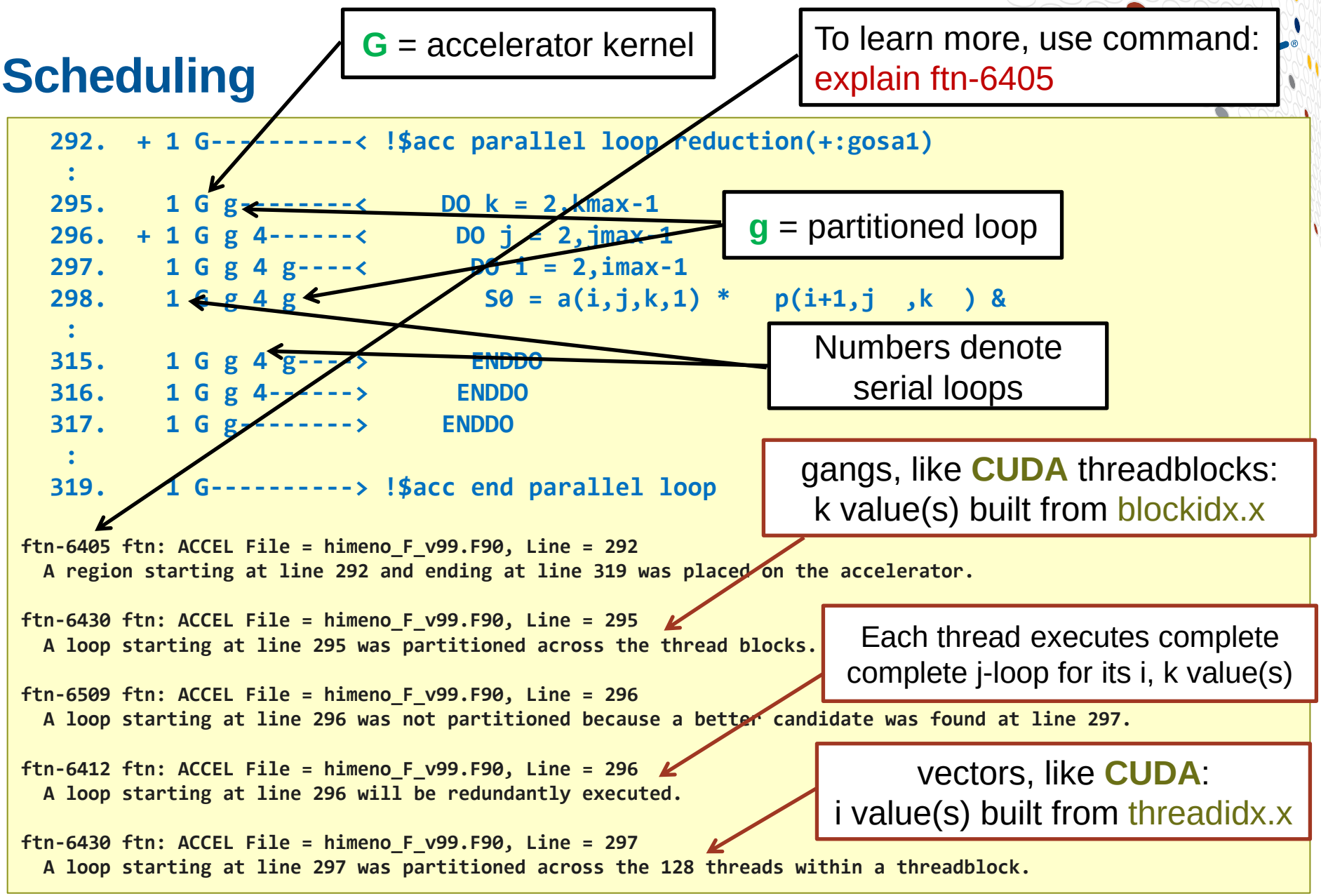
- copy* data clauses
  - compiler will do automatic analysis
    - usually correct
    - but can be over-cautious
- ***advice:***
  - *only use clauses if compiler over-cautious*
  - explicit data clauses will interfere with data directives at next step

```
gosa1 = 0d0

!$acc parallel loop reduction(+:gosa1) &
!$acc&  private(i,j,k,so,ss) &
!$acc&  copyin(p,a,b,c,bnd,wrk1) &
!$acc&  copyout(wrk2)
DO k = 2,kmax-1
 DO j = 2,jmax-1
  DO i = 2,imax-1
   s0 = a(i,j,k,1) * p(i+1,j, k ) &
     <etc...>

   ss = (s0*a(i,j,k,4) - p(i,j,k)) * &
                              bnd(i,j,k)
   gosa1 = gosa1 + ss*ss
   wrk2(i,j,k) = p(i,j,k) + omega*ss
  ENDDO
 ENDDO
ENDDO
!$acc end parallel loop
```

Compiler feedback

- **Compiler feedback is extremely important**
  - Did the compiler recognise the accelerator directives?
    - A good sanity check
  - How will the compiler move data?
    - Only use data clauses if the compiler is over-cautious on the copy*
    - Or you want to declare an array to be scratch space (create clause)
    - First major code optimisation: removing unnecessary data movements
  - How will the compiler schedule loop iterations across GPU threads?
    - Did it parallelise the loopnests?
    - Did it schedule the loops sensibly?
    - The other main optimisation is correcting obviously-poor loop scheduling
- **Compiler teams work very hard to make feedback useful**
  - *advice: use it, it's free!* (i.e. no impact on performance to generate it)
    - CCE: -hlist=a Produces commentary files <stem>.lst
    - PGI: -Minfo Feedback to STDERR

Scheduling




```
  292.  + 1 G----------< !$acc parallel loop reduction(+:gosa1)
   :
  295.    1 G g-------<     DO k = 2,kmax-1
  296.  + 1 G g 4-----<       DO j = 2,jmax-1
  297.    1 G g 4 g---<         DO i = 2,imax-1
  298.    1 G g 4 g             S0 = a(i,j,k,1) *   p(i+1,j  ,k  ) &
   :
  315.    1 G g 4 g--->         ENDDO
  316.    1 G g 4----->       ENDDO
  317.    1 G g------->     ENDDO
   :
  319.    1 G----------> !$acc end parallel loop

ftn-6405 ftn: ACCEL File = himeno_F_v99.F90, Line = 292
  A region starting at line 292 and ending at line 319 was placed on the accelerator.

ftn-6430 ftn: ACCEL File = himeno_F_v99.F90, Line = 295
  A loop starting at line 295 was partitioned across the thread blocks.

ftn-6509 ftn: ACCEL File = himeno_F_v99.F90, Line = 296
  A loop starting at line 296 was not partitioned because a better candidate was found at line 297.

ftn-6412 ftn: ACCEL File = himeno_F_v99.F90, Line = 296
  A loop starting at line 296 will be redundantly executed.

ftn-6430 ftn: ACCEL File = himeno_F_v99.F90, Line = 297
  A loop starting at line 297 was partitioned across the 128 threads within a threadblock.
```

Data movements

```
  292.  + 1 G----------< !$acc parallel loop reduction(+:gosa1)
   :
  295.    1 G g--------<     DO k = 2,kmax-1
  296.  + 1 G g 4------<      DO j = 2,jmax-1
  297.    1 G g 4 g----<       DO i = 2,imax-1
  298.    1 G g 4 g             S0 = a(i,j,k,1) *   p(i+1,j  ,k  ) &
   :
  315.    1 G g 4 g---->       ENDDO
  316.    1 G g 4------>      ENDDO
  317.    1 G g-------->     ENDDO
   :
  319.    1 G----------> !$acc end parallel loop

ftn-6415 ftn: ACCEL File = himeno_F_v99.F90, Line = 292
  Allocate memory and copy variable "gosa1" to accelerator, copy back at line 319 (acc_copy).

ftn-6418 ftn: ACCEL File = himeno_F_v99.F90, Line = 292
  If not already present: allocate memory and copy whole array "p" to accelerator, free at line 319 (acc_copyin).

< same messages for: "a", "b", "c", "wrk1", "bnd" >

ftn-6416 ftn: ACCEL File = himeno_F_v99.F90, Line = 292
  If not already present: allocate memory and copy whole array "wrk2" to accelerator, copy back at line 319 (acc_copy).
```

yes, as we expected

Over-cautious: compiler worried about halos;
we should add the clause: copyout(wrk2)

Run the first accelerated kernel

- **Original performance:**
  - `Measurement:  Gosa  : 0.13797154081596327E-02`
  - `Measurement: MFLOPS  :  2853.7552548501367`
- **With one OpenACC kernel:**
  - `Measurement:  Gosa  : 0.13797154081596570E-02`
  - `Measurement: MFLOPS  :  1354.6002299205898`
- **First: the answer is still correct**
  - *Advice: make sure you have correctness checks*
    - *e.g. checksums, residuals, representative array values*
      - *try to use double precision for reduction variables (checksums, residuals)*
      - *even if the code is single precision*
  - Note you won't get bitwise reproducibility between CPU and GPU
    - different compilers are also likely to give different results

Run the first accelerated kernel

- **Why is this first OpenACC version is slower?**
- **First we look at the Cray runtime commentary**
  - An event-by-event record of application execution
- **To use it:**
  - Compile with CCE (no special options)
  - Set environment variable: `CRAY_ACC_DEBUG=2`
  - Run the executable
  - The commentary is written to STDERR

CRAY_ACC_DEBUG=2

```
<For every iteration we see the following>

ACC: Start transfer 10 items from himeno_F_v99.F90:292
ACC:       allocate, copy to acc 'a' (68427792 bytes)
ACC:       allocate, copy to acc 'b' (51320844 bytes)
ACC:       allocate, copy to acc 'bnd' (17106948 bytes)
ACC:       allocate, copy to acc 'c' (51320844 bytes)
ACC:       allocate, copy to acc 'p' (17106948 bytes)
ACC:       allocate, copy to acc 'wrk1' (17106948 bytes)
ACC:       allocate 'wrk2' (17106948 bytes)
ACC:       allocate reusable, copy to acc <internal> (8 bytes)
ACC:       allocate reusable, copy to acc <internal> (4 bytes)
ACC:       allocate reusable <internal> (1008 bytes)
ACC: End transfer (to acc 222390336 bytes, to host 0 bytes)
ACC: Execute kernel jacobi_$ck_L292_1 blocks:126 threads:128 async(auto) from himeno_F_v99.F90:292
ACC: Wait async(auto) from himeno_F_v99.F90:319
ACC: Start transfer 10 items from himeno_F_v99.F90:319
ACC:       free 'a' (68427792 bytes)
ACC:       free 'b' (51320844 bytes)
ACC:       free 'bnd' (17106948 bytes)
ACC:       free 'c' (51320844 bytes)
ACC:       free 'p' (17106948 bytes)
ACC:       free 'wrk1' (17106948 bytes)
ACC:       copy to host, free 'wrk2' (17106948 bytes)
ACC:       copy to host, done reusable <internal> (8 bytes)
ACC:       done reusable <internal> (4 bytes)
ACC:       done reusable <internal> (0 bytes)
ACC: End transfer (to acc 0 bytes, to host 17106956 bytes)
```

More profile information

- **We can use the NVIDIA Compute Profiler to learn more:**
  - Event-by-event timing information

- **To use it:**
  - Compile with CCE (no special options)
  - Set environment variable: `COMPUTE_PROFILE=1`
  - Run the executable
  - The commentary is written to file cuda_profile_0.log

- **Advice:**
  - Don't set both `CRAY_ACC_DEBUG` with `COMPUTE_PROFILE`

COMPUTE_PROFILE=1

```
<For every iteration we see the following>

method=[ memcpyHtoD ] gputime=[ 27222.977 ] cputime=[ 27571.473 ]
method=[ memcpyHtoD ] gputime=[ 20372.352 ] cputime=[ 20636.215 ]
method=[ memcpyHtoD ] gputime=[ 6538.752 ] cputime=[ 6867.797 ]
method=[ memcpyHtoD ] gputime=[ 20333.984 ] cputime=[ 20594.152 ]
method=[ memcpyHtoD ] gputime=[ 6538.912 ] cputime=[ 6867.491 ]
method=[ memcpyHtoD ] gputime=[ 6547.712 ] cputime=[ 6871.381 ]
method=[ memcpyHtoD ] gputime=[ 1.632 ] cputime=[ 8.488 ]
method=[ memcpyHtoD ] gputime=[ 0.928 ] cputime=[ 6.142 ]
method=[ jacobi_$ck_L292_1 ] gputime=[ 2079.296 ] cputime=[ 25.261 ] occupancy=[ 0.312 ]
method=[ memcpyDtoH ] gputime=[ 35016.480 ] cputime=[ 37985.234 ]
method=[ memcpyDtoH ] gputime=[ 2.464 ] cputime=[ 19.153 ]
```

Profiling with CrayPAT

- **We really need an application-wide view using CrayPAT**
  - rather than an event-by-event account

- **To use it:**
  - module load perftools
  - Rebuild the code
  - Instrument the executable using pat_build -w command
    - Option -w does tracing of accelerator operations)
    - Option -u would include tracing of CPU routines as well
  - Rerun the code
  - Process the information gathered with pat_report command

pat_build -w

```
Table 1:  Profile by Function Group and Function

 Time%  |     Time   | Imb.   |  Imb.   | Calls   |Group
        |            | Time   | Time%   |         | Function

 100.0% | 10.801079 |    -- |     -- |  917.0 |Total
|-------------------------------------------------------------------------
| 100.0% | 10.800891 |    -- |     -- |  516.0 |USER
||------------------------------------------------------------------------
||  86.0% |  9.293427 |    -- |     -- |  103.0 |jacobi_.ACC_COPY@li.292
||   7.8% |  0.838496 |    -- |     -- |    1.0 |main_
||   4.2% |  0.448701 |    -- |     -- |  103.0 |jacobi_.ACC_COPY@li.319
||   2.0% |  0.215345 |    -- |     -- |  103.0 |jacobi_.ACC_SYNC_WAIT@li.319
|=========================================================================

Table 2:  Time and Bytes Transferred for Accelerator Regions

  Host   | Host   |  Acc   | Acc Copy   | Acc Copy   | Events   |Calltree
 Time%   | Time   | Time   |       In   |      Out   |          |
         |        |        | (MBytes)   | (MBytes)   |          |

 100.0% | 9.963 | 9.935 |     21845 |      1680 |     515 |Total
|-----------------------------------------------------------------------------------
| 100.0% | 9.963 | 9.935 |     21845 |      1680 |     515 |main_
|        |       |       |           |           |         | jacobi_
3        |       |       |           |           |         |  jacobi_.ACC_REGION@li.292
||||-------------------------------------------------------------------------------
4|||  93.3% | 9.293 | 9.275 |     21845 |        -- |     103 |jacobi_.ACC_COPY@li.292
4|||   4.5% | 0.449 | 0.444 |        -- |      1680 |     103 |jacobi_.ACC_COPY@li.319
4|||   2.2% | 0.215 |    -- |        -- |        -- |     103 |jacobi_.ACC_SYNC_WAIT@li.319
|===================================================================================
```

Step 3: Optimising data movements

- **Within jacobi routine**
  - data-sloshing: all arrays copied to/from GPU at every loop iteration
- **Need to establish data region outside the iteration loop**
  - Then data can remain resident on GPU for entire call
    - reused for each iteration without copying to/from host
- **Must accelerate all loopnests processing the arrays**
  - Even if they takes negligible compute time,
  - must still accelerate for data locality
    - This can be a lot of work
      - Performance of the kernels is irrelevant
    - A major productivity win for OpenACC compared to low-level languages
      - You can accelerate a loopnest with one directive; usually no need for tuning
      - You don't have to handcode a new CUDA kernel

Step 3: Structure of the jacobi routine

- data region spans iteration loop
  - includes both CPU and accelerator code
  - need explicit data clauses
    - no automatic scoping
    - requires knowledge of app
  - enclosed kernels
    - if in same routine
      - no data clauses for these variables
    - if in different routine
      - use present clause for these variables
    - see earlier advice
- **wrk2** now a scratch array
  - does not need copying

```
SUBROUTINE jacobi(nn,gosa)

!$acc data copy(p) &
!$acc&     copyin(a,b,c,wrk1,bnd) &
!$acc&     create(wrk2)
   iter_lp: DO loop = 1,nn

      gosa = 0d0
! compute stencil: wrk2, gosa from p
!$acc parallel loop <clauses>
      <stencil loopnest>
!$acc end parallel loop

! copy back wrk2 into p
!$acc parallel loop
      <copy loopnest>
!$acc end parallel loop

   ENDDO iter_lp
!$acc end data

END SUBROUTINE jacobi
```

Improved performance

- **Original performance:**
  - `Measurement:  Gosa  : 0.13797154081596327E-02`
  - `Measurement: MFLOPS  :  2853.7552548501367`
- **With one OpenACC kernel:**
  - `Measurement:  Gosa  : 0.13797154081596570E-02`
  - `Measurement: MFLOPS  :  1354.6002299205898`
- **With a data region around the iterations:**
  - `Measurement:  Gosa  : 0.13797154081596570E-02`
  - `Measurement: MFLOPS  :  40656.6334569459`
- **The code is correct**
  - and much faster
  - To see why, rerun with CRAY_ACC_DEBUG=2

CRAY_ACC_DEBUG=2

```
<Start of data region>

ACC: Start transfer 7 items from himeno_F_v99.F90:280
ACC:       allocate, copy to acc 'a' (68427792 bytes)
ACC:       allocate, copy to acc 'b' (51320844 bytes)
ACC:       allocate, copy to acc 'bnd' (17106948 bytes)
ACC:       allocate, copy to acc 'c' (51320844 bytes)
ACC:       allocate, copy to acc 'p' (17106948 bytes)
ACC:       allocate, copy to acc 'wrk1' (17106948 bytes)
ACC:       allocate 'wrk2' (17106948 bytes)
ACC: End transfer (to acc 222390324 bytes, to host 0 bytes)

<For each loop iteration... (see next slide)>

<After iteration loop finishes, close of data region>

ACC: Wait async(auto) from himeno_F_v99.F90:340
ACC: Start transfer 7 items from himeno_F_v99.F90:340
ACC:       free 'a' (68427792 bytes)
ACC:       free 'b' (51320844 bytes)
ACC:       free 'bnd' (17106948 bytes)
ACC:       free 'c' (51320844 bytes)
ACC:       copy to host, free 'p' (17106948 bytes)
ACC:       free 'wrk1' (17106948 bytes)
ACC:       free 'wrk2' (17106948 bytes)
ACC: End transfer (to acc 0 bytes, to host 17106948 bytes)
```

CRAY_ACC_DEBUG=2 continued

```
<Start of data region... (see previous slide)>

<For each loop iteration>

ACC: Start transfer 3 items from himeno_F_v99.F90:293
ACC:       allocate reusable, copy to acc <internal> (8 bytes)
ACC:       allocate reusable, copy to acc <internal> (4 bytes)
ACC:       allocate reusable <internal> (1008 bytes)
ACC: End transfer (to acc 12 bytes, to host 0 bytes)
ACC: Execute kernel jacobi_$ck_L293_1 blocks:126 threads:128 async(auto) from himeno_F_v99.F90:293
ACC: Wait async(auto) from himeno_F_v99.F90:320
ACC: Start transfer 3 items from himeno_F_v99.F90:320
ACC:       copy to host, done reusable <internal> (8 bytes)
ACC:       done reusable <internal> (4 bytes)
ACC:       done reusable <internal> (0 bytes)
ACC: End transfer (to acc 0 bytes, to host 8 bytes)
ACC: Execute kernel jacobi_$ck_L322_2 blocks:126 threads:128 async(auto) from himeno_F_v99.F90:322

<After iteration loop finishes, close of data region... (see previous slide)>
```

Profiling this version

- Why is this version going so much faster?
- We can generate a CrayPAT profile as before:

```
Table 1:  Profile by Function Group and Function

 Time%  |    Time  | Imb.  |  Imb.  | Calls  |Group
        |          | Time  | Time%  |        | Function

 100.0% | 0.755941 |    -- |     -- | 1131.0 |Total
|-------------------------------------------------------------------------
| 100.0% | 0.755749 |    -- |     -- |  730.0 |USER
||------------------------------------------------------------------------
||  40.9% | 0.308847 |    -- |     -- |    1.0 |main_
||  28.4% | 0.214851 |    -- |     -- |  103.0 |jacobi_.ACC_SYNC_WAIT@li.320
||  24.1% | 0.182321 |    -- |     -- |    2.0 |jacobi_.ACC_COPY@li.280
||   4.3% | 0.032620 |    -- |     -- |  103.0 |jacobi_.ACC_COPY@li.293
||   1.0% | 0.007862 |    -- |     -- |    2.0 |jacobi_.ACC_COPY@li.340
|=========================================================================

Table 2:  Time and Bytes Transferred for Accelerator Regions (see next slide)
```

A synchronous profile

- **GPU kernels launch asynchronously**
  - So the compute time shows up in the SYNC_WAIT events
- **We can switch off the automatic asynchronicity**
  - This can give a clearer profile, but it may be skewed
  - Recompile with CCE flag -hacc_model=auto_async_none
  - And do a new CrayPAT profile

pat_build -w, with auto_async_none

```
Table 1:  Profile by Function Group and Function

 Time%  |    Time  | Imb.  |  Imb.  | Calls  |Group
        |          | Time  | Time%  |        | Function

 100.0% | 0.756016 |    -- |     -- | 1026.0 |Total
|-----------------------------------------------------------------------
| 100.0% | 0.755826 |    -- |     -- |  625.0 |USER
||----------------------------------------------------------------------
||  40.7% | 0.307802 |    -- |     -- |    1.0 |main_
||  28.7% | 0.216719 |    -- |     -- |  103.0 |jacobi_.ACC_KERNEL@li.293
||  24.1% | 0.182522 |    -- |     -- |    2.0 |jacobi_.ACC_COPY@li.280
||   4.4% | 0.033479 |    -- |     -- |  103.0 |jacobi_.ACC_KERNEL@li.322
||   1.1% | 0.008124 |    -- |     -- |    2.0 |jacobi_.ACC_COPY@li.340
|=======================================================================

Table 2:  Time and Bytes Transferred for Accelerator Regions (see next slide)
```

pat_build -w, with auto_async_none (2)

```
Table 1:  Profile by Function Group and Function (see previous slide)

Table 2:  Time and Bytes Transferred for Accelerator Regions

  Host   | Host   |  Acc   | Acc Copy   | Acc Copy   | Events   |Calltree
 Time%   | Time   | Time   |       In   |      Out   |          |
         |        |        | (MBytes)   | (MBytes)   |          |

 100.0% | 0.448 | 0.437 |   424.177 |    32.630 |     624 |Total
|-------------------------------------------------------------------------------
| 100.0% | 0.448 | 0.437 |   424.177 |    32.630 |     624 |main_
|        |       |       |           |           |         | jacobi_
3        |       |       |           |           |         |  jacobi_.ACC_DATA_REGION@li.280
||||-----------------------------------------------------------------------------
4|||  49.9% | 0.224 | 0.217 |     0.001 |     0.001 |     412 |jacobi_.ACC_REGION@li.293
5|||  48.4% | 0.217 | 0.214 |        -- |        -- |     103 | jacobi_.ACC_KERNEL@li.293
4|||  40.7% | 0.183 | 0.180 |   424.176 |        -- |       2 |jacobi_.ACC_COPY@li.280
4|||   7.5% | 0.034 | 0.031 |        -- |        -- |     206 |jacobi_.ACC_REGION@li.322
5|||   7.5% | 0.034 | 0.031 |        -- |        -- |     103 | jacobi_.ACC_KERNEL@li.322
4|||   1.8% | 0.008 | 0.008 |        -- |    32.629 |       2 |jacobi_.ACC_COPY@li.340
|===============================================================================
```

Step 4: Further optimising data movements

- **The code times the calls to jacobi() routine**
- **Each call contains a data region**
  - So we are still timing some data movements
- **Solution: move up the call tree to parent routine**
  - Add a second, outer data region
    - Spans calls to iteration routines
  - Specified arrays then only move on boundaries of outer data region
  - moves the data copies outside of the timed region

Adding a data region

- Spans both calls to jacobi
  - plus timing calls
- Arrays just copyin now
  - and transfers not timed
  - **wrk2** could be create
- Keep data region in jacobi
  - you can nest data regions
  - arrays now declared present on inner region
  - could be copy_or_present
    - *advice: use present*
    - runtime error if not present
    - rather than just wrong result
- Drawback: arrays have to be in scope for this to work
  - may need to unpick clever use of module data
  - or use OpenACC v2.0 unstructured data regions

```
PROGRAM himeno
   CALL initmt

!$acc data copyin(p,a,b,c,bnd,wrk1,wrk2)
   cpu0 = gettime()
   CALL jacobi(3,gosa)
   cpu1 = gettime()

   cpu0 = gettime()
   CALL jacobi(nn,gosa)
   cpu1 = gettime()
!$acc end data

   END PROGRAM himeno
```

```
SUBROUTINE jacobi(nn,gosa)

!$acc data present(p,a,b,c,wrk1,bnd,wrk2)
   iter_lp: DO loop = 1,nn
     <...>
   ENDDO iter_lp
!$acc end data

END SUBROUTINE jacobi
```

Step 4: Going further

- **Best solution is to port entire application to GPU**
  - data regions span entire use of arrays
  - all enclosed loopnests accelerated with OpenACC
  - no significant data transfers

- **Expand outer data region**
  - to include call to initialisation routine as well
  - arrays can now all be declared as scratch space with create clause
  - need to accelerated loopnests in initmt(), declaring arrays present

- **N.B. No easy way to ONLY allocate arrays in GPU memory**
  - CPU version is now dead space, but
  - GPU memory is usually the limiting factor, so usually not a problem
  - Can use OpenACC API calls to do this, if really want to
    - Means more OpenACC-specific code changes

Porting entire application

- No significant data transfers now
  - doesn't improve measured performance in this case

```
PROGRAM himeno

!$acc data create(p,a,b,c,bnd,wrk1,wrk2)
   CALL initmt

   CALL jacobi(3,gosa)  ! plus timing calls

   CALL jacobi(nn,gosa) ! plus timing calls

!$acc end data

   END PROGRAM himeno
```

```
SUBROUTINE initmt
!$acc data present(p,a,b,c,wrk1,bnd)
!$acc parallel loop
   <set all elements to zero>

!$acc parallel loop
   <set some elements to be non-zero>
!$acc end data

END SUBROUTINE initmt
```

Add outer data region

- **Original performance:**
  - `Measurement:  Gosa  : 0.13797154081596327E-02`
  - `Measurement: MFLOPS  :  2853.7552548501367`
- **With one OpenACC kernel:**
  - `Measurement:  Gosa  : 0.13797154081596570E-02`
  - `Measurement: MFLOPS  :  1354.6002299205898`
- **With an inner data region around the iterations:**
  - `Measurement:  Gosa  : 0.13797154081596570E-02`
  - `Measurement: MFLOPS  :  40656.6334569459`
- **With an outer data region outside the timers**
  - `Measurement:  Gosa  : 0.13797154081596570E-02`
  - `Measurement: MFLOPS  :  56156.609816492906`

pat_build -w , with auto_async_none

```
Table 1:  Profile by Function Group and Function

 Time%  |    Time  | Imb.  |  Imb.  | Calls  |Group
        |          | Time  | Time%  |        | Function

 100.0% | 0.263683 |    -- |     -- | 1140.0 |Total
|-------------------------------------------------------------------------
|  99.9% | 0.263520 |    -- |     -- |  739.0 |USER
||------------------------------------------------------------------------
||  81.8% | 0.215700 |    -- |     -- |  103.0 |jacobi_.ACC_SYNC_WAIT@li.320
||  13.9% | 0.036764 |    -- |     -- |  103.0 |jacobi_.ACC_COPY@li.293
||   1.4% | 0.003685 |    -- |     -- |  103.0 |jacobi_.ACC_COPY@li.320
|=========================================================================

Table 2:  Time and Bytes Transferred for Accelerator Regions (see next slide)
```

pat_build -w , with auto_async_none (2)

```
Table 1:  Profile by Function Group and Function (see previous slide)

Table 2:  Time and Bytes Transferred for Accelerator Regions

  Host   | Host   |  Acc   | Acc Copy   | Acc Copy   | Events   |Calltree
 Time%   | Time   | Time   |       In   |      Out   |          |
         |        |        | (MBytes)   | (MBytes)   |          |

 100.0% | 0.264 | 0.255 |     0.001 |     0.001 |     738 |Total
|-------------------------------------------------------------------------------------
| 100.0% | 0.264 | 0.255 |     0.001 |     0.001 |     738 |main_
|        |       |       |           |           |         | main_.ACC_DATA_REGION@li.116
3  98.9% | 0.261 | 0.249 |     0.001 |     0.001 |     727 |  jacobi_
4        |       |       |           |           |         |   jacobi_.ACC_DATA_REGION@li.280
5  98.1% | 0.259 | 0.218 |     0.001 |     0.001 |     515 |    jacobi_.ACC_REGION@li.293
||||||-------------------------------------------------------------------------------
6|||||  81.8% | 0.216 |    -- |        -- |        -- |     103 |jacobi_.ACC_SYNC_WAIT@li.320
6|||||  14.0% | 0.037 | 0.001 |     0.001 |        -- |     103 |jacobi_.ACC_COPY@li.293
6|||||   1.4% | 0.004 | 0.002 |        -- |     0.001 |     103 |jacobi_.ACC_COPY@li.320
|===============================================================================
```

Elimination of data transfers

- **The remaining data transfers are small compiler internals**
  - associated with the reduction variables
  - and you have no control over these
  - so you shouldn't worry about them
    - if these really are the limiting factor in your application, well done!
- **To check this**
  - Use the CCE runtime commentary
  - Re-run with CRAY_ACC_DEBUG=2

OpenACC and/or OpenMP (more advanced)

- **GPU speed-up:**
  - 20x compared to a single core of the CPU
- **This is an unfair comparison**
  - full accelerator versus single CPU core
- **Run an OpenMP version to fully exercise CPU**
- **Overall GPU speedup compared to CPU: 3-5x**
  - This is the sort of figure we expect
    - Kepler GPU memory bandwidth around 5x compared to typical CPU

In summary

- **We ported the entire Himeno code to the GPU**
  - chiefly to avoid data transfers
    - 4 OpenACC kernels (only 1 significant for compute performance)
    - 1 outer data region
    - 2 inner data regions (nested within this)
  - 7 directive pairs for 200 lines of Fortran/C
  - Profiling frequently showed the bottlenecks
  - Correctness was also frequently checked

- **First step was optimising data transfers**

- **Next steps**
  - Checking kernels are scheduling sensibly
  - Look at kernel optimisation

In summary... continued

- **Further performance tuning**
  - data region gave a 20-40x speedup; kernel tuning is secondary
  - Low-level languages like CUDA
    - offer more direct control of the hardware
    - but OpenACC is much easier to use
      - should get close to CUDA performance
  - Remember Amdahl's Law:
    - speed up the compute of a parallel application,
      - and soon become network bound
    - Don't waste time trying to get an extra 10% in the compute
    - You are better concentrating your efforts on tuning the comms or I/O

- **Bottom line:**
  - 3-5x speedup from 7 directive pairs in 200 lines of Fortran/C
    - performance comparing GPU to the complete CPU

OpenACC 3: Performance Tuning

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Contents

- **How kernels execute on a GPU**
- **Scheduling**
  - the importance of vectorisation
  - the vector_length clause
  - tuning the schedule: collapse and worker clauses
  - further tuning: cache and tile

The next step

- **Once data movements have been optimised**
  - the next step is to improve the kernel scheduling
    - understand how the iterations of the loopnest are divided between threads
      - This is called "partitioning" of the loops
    - and how the threads are executed on the hardware
  - then we can improve this scheduling
- **For this, we need to understand how the hardware works**
  - we'll concentrate on Nvidia GPUs for this

How a kernel is executed on a GPU

- **A GPU kernel is executed by a large pool of threads**
  - Whether we use OpenACC or CUDA
  - The threads are logically divided into sets called threadblocks
  - Each threadblock executes on a different piece of hardware
    - Symmetric Multiprocessor (SM)
    - (Almost) like a single vector processor

- **Within a threadblock**
  - The threads are logically divided into sets called warps
    - threads within a warp (32 threads) are executed concurrently
    - (almost) like a set of vector instructions, each of fixed width 32
  - so the threadblock executes as a sequence of concurrent warps

- **The CUDA programming model**
  - does not make warps explicit
  - but you need to know about them to understand code performance

OpenACC scheduling

- **OpenACC makes the distinction explicit**
  - gang is the same as threadblock (just as in CUDA)
  - worker refers to an entire warp
    - i.e. entire width-32 vector instructions (32 is fixed by the hardware)
  - vector refers to threads within a warp
    - i.e. 32 threads that do the same thing at the same time
- **When a loopnest is partitioned by the compiler**
  - The loop iterations are divided up into gangs of workers
    - each worker executes sets of vector instructions (warps)
  - There are many different ways for the compiler to do this
    - If you give no further instruction, the compiler will make a decision
    - You can see what this was from the compiler feedback
    - You can then over-ride this decision (at the next compilation)
      - by adding additional OpenACC directives and clauses
- **This is one place where OpenACC differs from OpenMP**
  - OpenMP parallel regions only partition one loop over the CPU threads
  - OpenACC parallel/kernels regions partition up to three nested loops

Kernel vectorisation

- **After minimising data movements, next optimisation:**
  - make sure all the kernels vectorise
  - meaning the compiler is efficiently using vector instructions on GPU

- **How can I tell if there is a problem?**
  - if a kernel is surprisingly slow on accelerator
    - in a very-different place in the profile compared to running on CPU
  - then examine the compiler commentary
    - CCE: compile with flag -hlist=a to generate *.lst loopmark file

- **Should see loop iterations divided both:**
  - over threads within a threadblock (vector) and
  - over threadblocks (gang)

Vectorisation and loopmark

- **With CCE, you should see:**
  - For a single loop:
    - should be divided over both levels of parallelism
    - look for this in the loopmark: Gg
  - For a loopnest:
    - Two (or maybe three) loops should be "partitioned" (divided):
    - look for G and 2 (or maybe 3) g-s
      - possibly with some numbers in between

```
171. 1 G-----<> !$acc parallel loop ...
172. 1 g-----<   DO k = 2,kmax-1
173. 1 g 3---<     DO j = 2,jmax-1
174. 1 g 3 g-<       DO i = 2,imax-1
175. 1 g 3 g           s0 = a(i,j,k,1) * p(i+1,j,k) ...
188. 1 g 3 g->       ENDDO
189. 1 g 3--->     ENDDO
190. 1 g----->   ENDDO
191. 1           !$acc end parallel loop
```

A loop starting at line 172 was partitioned across the thread blocks.

A loop starting at line 174 was partitioned across the 128 threads within a threadblock.

Kernel optimisation

- **Making sure all the kernels vectorise**
  - should have one loop "partitioned across threads within a threadblock"
- **Which loop do we want to vectorise?**
  - generally want to vectorise the innermost loop
  - usually labels fastest-moving array index, for coalescing
- **If it is not vectorised, can we make it vectorise?**
  - Can loop iterations be computed in any order?
    - No? Then can we rewrite code
      - avoid loop-carried dependencies
      - e.g. buffer packing: calculate rather than increment
      - these rewrites will probably perform better on CPU
      - there is a lot of literature on vectorisable algorithms

Replace:

```
i = 0
DO y = 2,N-1
   i = i+1
   buffer(i) = a(2,y)
ENDDO
buffsize = i
```

By:

```
DO y = 2,N-1
   buffer(y-1) = a(2,y)
ENDDO
buffsize = N-2
```

Forcing compiler to vectorise

- **Can loop iterations be computed in any order?**
  - Yes? Then we should guide the compiler
  - Either with a gentle hint:
    - put "acc loop independent" directive above this loop
      - recompile the routine and check compiler feedback to see if this worked
  - Or with a direct order:
    - put "acc loop vector" directive above this loop
  - check the code is still correct (as well as running faster)
    - the compiler might not be vectorising the loop for a good reason
- **Advice:**
  - Remember to repeat any reduction clauses on new loop directives

Changing the vectorisation with seq

- **If the inner loop is vectorising but performance is still bad**
  - Is the inner loop really the one to vectorise in this case?
    - in this example, we should vectorise the i-loop
      - because we happen to know mmax is small here
      - or because CrayPAT loop-level profiling told us this
  - Put "acc loop seq" directive above m-loop
    - then executed "redundantly" by every thread
    - also t is now an i-loop private scalar
      - rather than a reduction variable
      - this should also help performance

```
!$acc parallel loop
DO i = 1,N
   t = 0
!$acc loop seq
   DO m = 1,mmax
      t = t + c(m,i)
   ENDDO
   a(i) = t
ENDDO
!$acc end parallel loop
```

- **The compiler should now vectorise a different loop**
  - usually the next one up in the loopnest
    - in this case there is no choice but the i-loop
  - if it is not the next one up in the loopnest
    - you will need to put an "acc loop vector" directive in the right place

An aside on this example

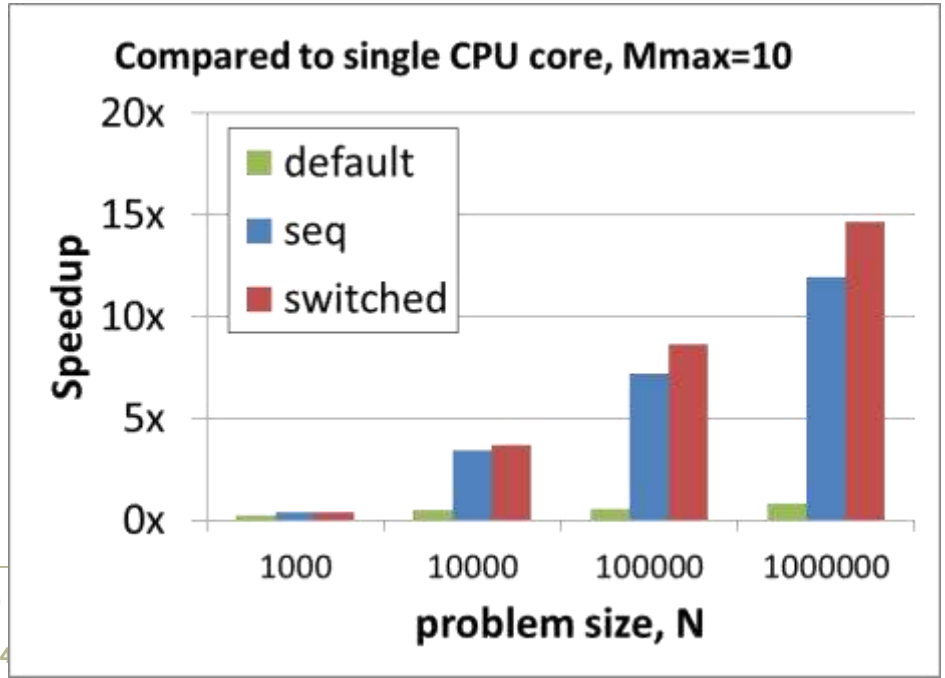
- **We forced vectorisation of the i-loop**
  - because mmax was too small
    - small loops will not give the GPU enough work
- **Performance is still likely to be bad**
  - a warp is 32 threads, executing as a vector
    - each thread has a different i-value
  - data for the warp is done in vector loads
    - but c(m,1:32) is not a contiguous chunk of memory
    - so we will need multiple vector loads for each warp
  - loads/stores from global memory are slow, so performance will suffer
    - this is a hardware feature, not a limitation of OpenACC

```
!$acc parallel loop
DO i = 1,N
   t = 0
!$acc loop seq
   DO m = 1,mmax
      t = t + c(m,i)
   ENDDO
   a(i) = t
ENDDO
!$acc end parallel loop
```

More aside on this example

- **So what can we do?**
  - Re-arrange the affected data arrays to allow coalescing
    - so warps get their data in the minimum number of vector loads/stores
  - We want the vector index to be fastest-moving array index
    - switched array ct(i,m) now gives coalesced memory accesses
    - because ct(1:32,m) is a contiguous chunk of memory
  - But this does mean refactoring your code
    - which may (or may not) be much work
    - Note: you may also get better CPU performance (e.g. with AVX instructions)

```
!$acc parallel loop
DO i = 1,N
   t = 0
!$acc loop seq
   DO m = 1,mmax
      t = t + ct(i,m)
   ENDDO
   a(i) = t
ENDDO
!$acc end parallel loop
```



It's all vectorising, but still performing badly

- **Profile the code and start where it takes most time**
  - check the slowest thing really is compute kernels
  - if it really is a GPU compute kernels...
- **GPUs need lots of parallel tasks to work well**
  - check that there really are enough loop iterations
- **Then look at loop scheduling using OpenACC clauses**
- **Then might need to consider more extreme measures**
  - source code changes
  - handcoding CUDA kernels

Tuning the partitioning

- **Before we alter the schedule, two easy tuning choices**
  - number of threads per threadblock; total number of threadblocks
- **Do this with clauses on the parallel/kernels directives**
- **vector_length(<value>)**
  - changes the number of threads per threadblock
  - CCE-specific details:
    - value needs to be fixed at compile time
    - allowed values are: 1, 32, 64, 128, 256, 512, 1024
    - default value is 128
- **num_gangs(<value>)**
  - changes the number of threadblocks
  - you do not have to specify this (unlike with CUDA)
  - the compiler will make a default choice of sufficient blocks

Over-riding the default scheduling

- **You can change how loops are scheduled**
  - by adding additional loop directives above the relevant loops
    - with clauses to tell the compiler how to schedule that loop
  - use clauses: gang, worker, vector
    - we've already seen vector in use in the previous example
  - you can also use the seq clause
    - tells compiler what not to do, allowing it freedom in scheduling remaining loops
- **Can partition a loop over multiple levels of parallelism**
  - Put more than one of gang, worker, vector clauses on loop directive
  - To schedule one loop over whole device:
    - acc loop gang worker vector

Over-riding the default scheduling

- **You can only mention gang, worker, vector (at most) once each per kernel**
  - any not mentioned will be handled automatically by the compiler
    - it will choose where best to apply them
  - once all levels of parallelism are used up
    - additional loops will execute sequentially (redundantly)

- **Handy tip:**
  - To debug a kernel by running on a single GPU thread, use:
    - !$acc parallel loop gang worker vector num_gangs(1) vector_length(1)
  - Useful for checking race conditions in parallelised loopnests
    - but execution will be very slow, so maybe find a cut-down testcase first

Aside: vector_length bigger than 32?

- What happens if vector_length is larger than 32?
- Warps execute vector instructions of width 32
  - this is fixed by the hardware)
- If vector_length is more than 32
  - multiple vector instructions are used to implement the operations
  - i.e. each vector is decomposed into multiple warps
    - or multiple workers, in the language of OpenACC
- This is exactly what happens under-the-hood in CUDA

Advanced loop scheduling

- **OpenACC loop schedules are limited by the loop bounds**
  - one loop's iterations are divided over threadblocks
  - another loop's iterations are divided over threads in threadblock

- **This has limitations, for instance**
  - "tall, skinny" loopnests (j=1:big; i=1:small) won't schedule well
    - inner loop is too small
      - if less than 32 iterations won't even fill a warp, so wasted SIMT
  - "short, fat" loopnests (j=1:small; i=1:big) also not good
    - outer loop is too small
      - want lots of threadblocks to swap amongst SMs

  - In both cases there are enough total iterations to keep the GPU busy
    - but division of iterations between the two loops is non-optimal for the GPU

- **How do we better spread the loop iterations over the GPU?**
  - collapse clause
  - worker clause

collapse clause

- **A way of increasing OpenACC scheduling flexibility**
- **Merges iterations of two or more loops together**
  - We then apply OpenACC scheduling clauses to the composite loop
  - Both "tall, skinny" and "short, fat" examples will benefit from
    - acc loop collapse(2) gang worker vector
      - collapse the j and i loops into a single iteration space
        - effectively the same as DO ij=1,small*big
      - then divide the total iterations over all levels of parallelism on the GPU
  - Things to look for
    - the compiler may use this automatically (look for C in loopmark feedback)
    - no guarantee that it is faster
      - index rediscovery (if needed) uses expensive integer divisions
        - e.g. j = INT(ij/big); i = ij - j*big
    - you can only collapse perfectly nested loops
  - The next slides give some examples of using the clause

Examples of using the collapse clause

- **Consider a three-level loopnest**
  - must be perfectly nested for collapse clause

```
DO k = 1,Nk
  DO j = 1,Nj
    DO i = 1,Ni
```

- **Here are a few examples of what you might do:**
  - Collapse all loops and schedule across GPU
    - "gang worker vector" optional here
      - there's only one composite loop left to partition
    - Small tripcount loops benefit from this
      - better division of iterations

```
!$acc parallel loop &
!$acc collapse(3) &
!$acc gang worker vector
DO k = 1,Nk
  DO j = 1,Nj
    DO i = 1,Ni
```

  - Schedule inner two loops over threadblock
    - "gang" optional here
    - Good if k-loop is quite large, but i-loop small
      - but you often see that collapse(3) is better

```
!$acc parallel loop &
!$acc gang
DO k = 1,Nk
!$acc loop collapse(2) &
!$acc vector
  DO j = 1,Nj
    DO i = 1,Ni
```

More examples using the collapse clause

- **Here are a few more examples of what you might do:**
  - Usually these don't give the best performance
  - Schedule outer two loops over threadblocks
    - "acc loop vector" optional here

```
!$acc parallel loop &
!$acc collapse(2) gang
DO k = 1,Nk
  DO j = 1,Nj
!$acc loop vector
    DO i = 1,Ni
```

  - Schedule outer two loops over entire GPU
    - "acc loop seq" optional here

```
!$acc parallel loop &
!$acc collapse(2) &
!$acc gang worker vector
DO k = 1,Nk
  DO j = 1,Nj
!$acc loop seq
    DO i = 1,Ni
```

  - Schedule k,i-loops together over entire GPU
    - i.e. you want to collapse just the i- and k-loops
    - you can't:
      - collapsed loops must be perfectly nested (i.e. consecutive statements in the code)
      - so you'll need to reorder the loops in the code first

Explicit worker clauses

- **We've already seen the worker clause**
  - as part of "gang worker vector", meaning "everything"
- **Often, the compiler partitions two loops**
  - the outermost loop over gangs
  - the innermost loop over vector
  - remaining loops are executed redundantly (sequentially) by all threads
  - if the innermost loop has more than 32 iterations
    - it is automatically split into multiple workers
- **We can use the worker clause to partition a third loop**
  - Doesn't change the total work (number of loopnest iterations)
  - But does change how work distributed between threads

collapse or worker?

- **Both try to increase the scheduling flexibility**
- **Perfectly nested loops with one or more low tripcounts**
  - probably better to use the collapse clause
- **Imperfectly nested loops with one or more low tripcounts**
  - may benefit to put "!$acc loop worker" on the middle loop
    - collapse won't work here
- **But it is difficult to predict which will be best**
  - You may need to try both

The cache directive

- **Main accelerator memory is relatively slow**
  - If a data element is accessed multiple times
  - It may make sense to temporarily store it in a faster cache
  - typical use case is a finite difference stencil, e.g.
    - for all `i`, calculate: `a[i]=b[i+1]-2*b[i]+b[i-1]`
      - `b[3]` is used three times, to calculate all of: `a[2]`, `a[3]`, `a[4]`.
    - so we would like to cache values of `b` for reuse by other loop iterations

- **The cache directive suggests this to the compiler**
  - suggests, but does not compel: compiler can ignore suggestion
    - e.g. if you try to store more data than the cache can hold
    - check compiler feedback to see what it did
  - No guarantee that this improves performance
    - you may be polluting some automatic caching (hardware or software)

- **Nvidia GPUs**
  - threads within a threadblock execute on single SM piece of hardware
  - have joint access to a common, fast, but small, "shared memory"

cache clause example

- **A first example:**
  - loop-based stencil
    - bigger than before
    - size: 2*RADIUS+1
  - inner loop must be sequential
  - RADIUS should be known at compile time (parameter or cpp)

```
!$acc parallel loop copyin(c)
  DO i = 1,N
   result = 0
!$acc cache(in(i-RADIUS:i+RADIUS),c)
!$acc loop seq
   DO j = -RADIUS,RADIUS
    result = result + c(j)*in(i+j)
   ENDDO
   out(i) = result
  ENDDO
```

Multi-dimensional loopnests

- **How much data should be cached here?**
  - B(NI-1:NI+1,j,k) would probably fill the cache for one j,k value
  - And we wouldn't get any re-use for j±1

- **To use the cache clause here**
  - Need to tile the loopnest
  - The compiler may do this
  - Or we may want more explicit control

```
!$acc parallel loop
DO k = 1,Nk

  DO j = 1,Nj
    DO i = 1,Ni
!$acc cache( B(i-1:i+1,j-1:j+1,k) )

      A(i,j,k) = B(i,  j,  k) - &
                 ( B(i-1,j-1,k) &
                 + B(i-1,j+1,k) &
                 + B(i+1,j-1,k) &
                 + B(i+1,j+1,k) ) / 5
    ENDDO
  ENDDO
ENDDO
!$acc end parallel
```

The tile clause

- Added to loop directive (new for OpenACC 2.0)
- Used to block loops in a loopnest
- Two main use cases:
- To help the compiler implement the cache directive
  - Inner "element" loops have a fixed tripcount
  - So compiler knows how much shared memory is needed for cache
- To allow compiler to use multidimensional threadblocks

The tile clause in more detail

- **Blocks loops in a loopnest**
  - Using specified blocking factors
    - fixed at compile-time
    - Or * to use compiler default
    - one argument per loop
  - Outer tile loops
    - migrated to outside of nest
  - Inner element loops
    - have known size

```
!$acc loop tile(8,16)  ! next 2 loops
DO j = 1,Nj
 DO i = 1,Ni
```

```
! equivalent explicit code
!$acc loop
DO jtile = 1,Nj,16
 DO itile = 1,Ni,8

  DO j = jtile,jtile+16-1
   DO i = itile,itile+8-1
```

- **Scheduling clauses on loop directive still apply, if used**
  - gang applies to outer, tile loops
  - vector applies to inner, element loops
    - probably want composite tilesize to be multiple of 32
  - worker might apply to either, depending on how used (see Standard)

Multi-dimensional caching

- **The explicit version:**
  - j-loop: tilesize=16
  - i-loop tilesize=64
  - automatic scheduling:
    - outer tile loops: worker
    - inner element loops: vector
  - cached data:
    - (64+2)*(16+2)=1188 elements
      - 4kB of floats or integers
      - 8kB of doubles

```
!$acc parallel loop gang
DO k = 1,Nk
!$acc loop tile(64,16) worker vector
  DO j = 1,Nj
    DO i = 1,Ni
!$acc cache( B(i-1:i+1,j-1:j+1,k) )

      A(i,j,k) = B(i,  j,  k) - &
                 ( B(i-1,j-1,k) &
                 + B(i-1,j+1,k) &
                 + B(i+1,j-1,k) &
                 + B(i+1,j+1,k) ) / 5
    ENDDO
  ENDDO
ENDDO
!$acc end parallel
```

Conclusions

- **Scheduling is the biggest optimisation**
  - after data movements
- **Does the code vectorise?**
  - Does it vectorise the right loop
- **Can collapsing loops help?**
- **Can workers help?**
- **Caching and tiling might be useful at the end**

Porting a larger code

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Adding OpenACC to a Larger Code

- **Adding OpenACC to a real code is not trivial work…**
  - Are parts of the program suitable for an accelerator?
  - Where do we start?
  - What do we do next?

- **We'll go through the exercise for an example code**
  - Running on a Cray XC30
  - Using Cray compiler and Cray performance analysis tools

The Code

- **NAS Parallel Benchmarks MG (MultiGrid) code**
  - Shorter than typical application
    - but structure of code is very similar
  - This example concentrates on the serial version
    - We also have parallel versions ported to OpenACC
    - The serial versions have OpenMP directives, but we do not use them during this exercise
  - Downloading it:
    - Fortran version: http://www.nas.nasa.gov/publications/npb.html.
      - 1445 lines, of which 267 blank
    - C version: http://www.hpcs.cs.tsukuba.ac.jp/omni-openmp/download/download-benchmarks.html.
      - 1292 lines, of which 206 blank

Building and Running MG

- **Run the code on the CPU:**
  - Three important lines of output
  - Fortran
    - `L2 Norm is  0.180056440135E-05`
    - `Mop/s total     =                  4787.41  ! Fortran`
    - `Verification    =                SUCCESSFUL`
  - C output same, but baseline performance differs
    - `Mop/s total     =                  4848.87  // C`

Where Do We Start?

- Profile MG on the CPU (standard CrayPAT report)

```
Table 1:  Profile by Function Group and Function

 Time%  |    Time  | Imb.  |  Imb.  | Calls  |Group
        |          | Time  | Time%  |        | Function

 100.0% | 4.213820 |    -- |     -- | 1630.0 |Total
|-------------------------------------------------------
| 100.0% | 4.213768 |    -- |     -- | 1230.0 |USER
||------------------------------------------------------
||  47.8% | 2.013292 |    -- |     -- |  161.0 |resid_
||  23.9% | 1.008719 |    -- |     -- |  160.0 |psinv_
||  14.2% | 0.599713 |    -- |     -- |  140.0 |rprj3_
||  10.7% | 0.450218 |    -- |     -- |  140.0 |interp_
||   2.1% | 0.089875 |    -- |     -- |  461.0 |comm3_
|=======================================================
```

- Four routines dominate the runtime
  - More than half the time is spent in **resid**
  - There are other routines executing for less than 1% of the total time
    - These might be important for the OpenACC port

Understand Flow of the Application

```
Table 1:  Function Calltree View

 Time%  |    Time  | Calls  |Calltree

 100.0% | 4.213820 | 1630.0 |Total
|-----------------------------------
| 100.0% | 4.213768 | 1230.0 |mg_
||----------------------------------
||  76.0% | 3.202582 | 1180.0 |mg3p_
|||---------------------------------
3||  25.5% | 1.074038 |  280.0 |resid_
3||  24.6% | 1.038074 |  320.0 |psinv_
3||  14.4% | 0.605792 |  280.0 |rprj3_
3||  10.7% | 0.450218 |  140.0 |interp_
|||=================================
||  23.6% | 0.993695 |   42.0 |resid_
|====================================
```

- **CrayPAT report with calltree**
- **mg calls:**
  - mg3p (which then calls resid, psinv, rprj3, interp)
  - resid also called directly from mg

Get Work Estimates for Loops

```
Table 2:  Loop Stats by Function (from -hprofile_generate)

    Loop  |   Loop  |   Loop  |  Loop  |  Loop  |Function=/.LOOP[.]
    Incl  |    Hit  |  Trips  | Trips  | Trips  |
    Time  |         |    Avg  |   Min  |   Max  |
   Total  |         |         |        |        |
|-------------------------------------------------------------------
| 2.073902 |     161 |  96.497 |      4 |    256 |resid_.LOOP.1.li.634
| 2.073579 |   15536 | 201.067 |      4 |    256 |resid_.LOOP.2.li.635
| 1.013344 | 3123776 | 235.548 |      4 |    256 |resid_.LOOP.4.li.642
| 0.972528 | 3123776 | 237.548 |      6 |    258 |resid_.LOOP.3.li.636
```

- **Loop-level profiling is more useful now**
  - Which loopnests (rather than just routines) took most time?
  - How may iterations did this loopnest have?
- **Here are the lines relating to resid**
  - Loops starting at 636 and 642 are nested inside loops at line 634, 635
    - See how the Loop Hit numbers multiply up
    - See how inclusive times for 636 and 642 add to give that for 635
    - Inclusive times for 634, 635 same: perfectly nested loops

Add First OpenACC Kernel

- **Clearly we should start with resid**
  - Fortran:

```
!$acc parallel loop &
!$acc private(u1,u2) &
!$acc copyin(u,v,a) &
!$acc copyout(r)
DO i3=2,n3-1
  DO i2=2,n2-1
    DO i1=1,n1
      u1(i1) = ...
      u2(i1) = ...
    ENDDO
    DO i1=2,n1-1
      r(i1,i2,i3) = v(i1,i2,i3)
```

  - C:
    - Data movement sizes explicit
    - to avoid "unshaped pointer" errors
    - Because dynamically allocating memory

```
#pragma acc parallel loop \
   private(u1,u2) \
   copyin(u[0:n1*n2*n3]) \
   copyin(v[0:n1*n2*n3]) \
   copyin(a[0:4]) \
   copyout(r[0:n1*n2*n3])
for (i3 = 1; i3 < n3-1; i3++) {
  for (i2 = 1; i2 < n2-1; i2++) {
    for (i1 = 0; i1 < n1; i1++) {
      <...>
```

Resulting MG Performance?

- Running with and without OpenACC kernel:

	Original (Mop/s)	1 kernel (Mop/s)
Fortran	4787	3509
C	4849	3597

- So the code is actually slower... **Why?**

Enable Cray Runtime Commentary

- export CRAY_ACC_DEBUG=2
- for every call to resid:

```
ACC: Start transfer 6 items from mg_v02.f:615
ACC:       allocate, copy to acc 'a' (32 bytes)
ACC:       allocate 'r' (137388096 bytes)
ACC:       allocate, copy to acc 'u' (137388096 bytes)
ACC:       allocate, copy to acc 'v' (137388096 bytes)
ACC:       allocate <internal> (530432 bytes)
ACC:       allocate <internal> (530432 bytes)
ACC: End transfer (to acc 274776224 bytes, to host 0 bytes)
ACC: Execute kernel resid_$ck_L615_1 blocks:256 threads:128 async(auto) from mg_v03.f:615
ACC: Wait async(auto) from mg_v02.f:639
ACC: Start transfer 6 items from mg_v02.f:639
ACC:       free 'a' (32 bytes)
ACC:       copy to host, free 'r' (137388096 bytes)
ACC:       free 'u' (137388096 bytes)
ACC:       free 'v' (137388096 bytes)
ACC:       free <internal> (0 bytes)
ACC:       free <internal> (0 bytes)
ACC: End transfer (to acc 0 bytes, to host 137388096 bytes)
```

- Certainly a lot of data was moved
  - Commentary tells us which arrays, at which line and how much data

Or Use Nvidia Compute Profiler

- **export COMPUTE_PROFILE=1**
  - Analyses PTX (from OpenACC or from CUDA)
  - Very useful if mixing OpenACC with CUDA code

```
method=[ memcpyHtoD ] gputime=[ 1.248 ] cputime=[ 6.727 ]
method=[ memcpyHtoD ] gputime=[ 23297.504 ] cputime=[ 23345.885 ]
method=[ memcpyHtoD ] gputime=[ 23329.568 ] cputime=[ 23329.770 ]
method=[ resid_$ck_L615_1 ] gputime=[ 7611.488 ] cputime=[ 16.093 ] occupancy=[ 0.312 ]
method=[ memcpyDtoH ] gputime=[ 63877.535 ] cputime=[ 64378.523 ]
```

- **Data transfers obvious, taking most time**

Or Use CrayPAT for a Profile by Function

```
Table 1:  Profile by Function Group and Function

 Time%  |    Time   | Imb.   |  Imb.   | Calls   |Group
        |           | Time   | Time%   |         | Function

 100.0% | 6.981196 |    -- |     -- | 1252.0 |Total
|-------------------------------------------------------------------------
| 100.0% | 6.981093 |    -- |     -- |  851.0 |USER
||------------------------------------------------------------------------
||  48.2% | 3.364813 |    -- |     -- |    1.0 |mg_
||  31.2% | 2.175330 |    -- |     -- |  170.0 |resid_.ACC_COPY@li.615
||  15.3% | 1.068125 |    -- |     -- |  170.0 |resid_.ACC_COPY@li.639
||   5.3% | 0.368549 |    -- |     -- |  170.0 |resid_.ACC_SYNC_WAIT@li.639
||   0.1% | 0.003585 |    -- |     -- |  170.0 |resid_.ACC_ASYNC_KERNEL@li.615
||   0.0% | 0.000691 |    -- |     -- |  170.0 |resid_.ACC_REGION@li.615
||========================================================================
|   0.0% | 0.000103 |    -- |     -- |  401.0 |ETC
||------------------------------------------------------------------------
```

- **Provides aggregated report of data movements**
  - names, sizes and frequencies of original arrays lost
- **Shows asynchronous kernel launches**
  - Notice ACC_KERNEL almost zero
  - SYNC_WAIT shows the compute time
  - could recompile with -hacc_model=auto_async_none

…And CrayPAT Accelerator Statistics

```
Table 2:  Time and Bytes Transferred for Accelerator Regions

  Host  | Host  |  Acc  | Acc Copy  | Acc Copy  | Events  |Calltree
 Time%  | Time  | Time  |       In  |      Out  |         |
        |       |       | (MBytes)  | (MBytes)  |         |

 100.0% | 8.007 | 7.962 |     12341 |      6171 |     850 |Total
|-------------------------------------------------------------------------------------------
| 100.0% | 8.007 | 7.962 |     12341 |      6171 |     850 |mg_
||------------------------------------------------------------------------------------------
||  50.0% | 4.005 | 3.969 |      6314 |      3157 |     735 |mg3p_
3|        |       |       |           |           |         | resid_
4|        |       |       |           |           |         |  resid_.ACC_REGION@li.615
|||||----------------------------------------------------------------------------------------
5||||  36.2% | 2.898 | 2.877 |      6314 |        -- |     147 |resid_.ACC_COPY@li.615
5||||  10.8% | 0.867 | 0.860 |        -- |      3157 |     147 |resid_.ACC_COPY@li.639
5||||   2.9% | 0.235 |    -- |        -- |        -- |     147 |resid_.ACC_SYNC_WAIT@li.639
5||||   0.1% | 0.004 | 0.232 |        -- |        -- |     147 |resid_.ACC_KERNEL@li.615
5||||   0.0% | 0.001 |    -- |        -- |        -- |     147 |resid_.ACC_REGION@li.615(exclusive)
```

- **Host and accelerator times given separately**
  - ACC_KERNEL
    - Acc Time is the compute time
    - Host Time is the time for the asynchronous launch
      - The Host "catches up" at the SYNC_WAIT

… And CrayPAT Summarized Trace

- pat_build -u mg.B.x

```
Table 1:  Profile by Function Group and Function

 Time%  |    Time  | Imb.  |  Imb.  |   Calls  |Group
        |          | Time  | Time%  |          | Function

 100.0% | 7.005544 |    -- |     -- | 265301.0 |Total
|-------------------------------------------------------------------------
| 100.0% | 7.005442 |    -- |     -- | 264900.0 |USER
||------------------------------------------------------------------------
||  31.1% | 2.176236 |    -- |     -- |    170.0 |resid_.ACC_COPY@li.615
||  15.2% | 1.067545 |    -- |     -- |    170.0 |resid_.ACC_COPY@li.639
||  15.2% | 1.066457 |    -- |     -- |    168.0 |psinv_
||  11.6% | 0.811638 |    -- |     -- | 131072.0 |vranlc_
||   9.1% | 0.637047 |    -- |     -- |    147.0 |rprj3_
||   6.7% | 0.469986 |    -- |     -- |    147.0 |interp_
||   5.3% | 0.368538 |    -- |     -- |    170.0 |resid_.ACC_SYNC_WAIT@li.639
||   1.5% | 0.103028 |    -- |     -- |    149.0 |zero3_
||   1.5% | 0.102412 |    -- |     -- |      2.0 |zran3_
||   1.4% | 0.098443 |    -- |     -- |    487.0 |comm3_
|=========================================================================
```

- resid kernel no longer dominates the profile
  - actual compute time is shown in SYNC_WAIT (Host) Time
  - Its data copies are significant, however

More OpenACC Kernels

- Running with 4 accelerated kernels:

	Original (Mop/s)	1 kernel (Mop/s)	4 kernels (Mop/s)
Fortran	4787	3509	2727
C	4849	3597	1727

- Even slower, and C particularly bad. **Why?**

Profile the Code Again

- Notice that spending most time in interp()
- Next look at compiler listing:

```
704.              #pragma acc parallel loop private(z1,z2,z3)  \
705.                copy(u[0:n1*n2*n3])                        \
706.                copyin(z[0:mm1*mm2*mm3])
707.  + gG--------<     for (i3 = 0; i3 < mm3-1; i3++) {
708.  + gG 2------<       for (i2 = 0; i2 < mm2-1; i2++) {
709.    gG 2 g----<         for (i1 = 0; i1 < mm1; i1++) {
710.    gG 2 g                i123 = i1 + mm1*i2 + mm12*i3;
711.    gG 2 g                  z1[i1] = z[i123+mm1] + z[i123];
712.    gG 2 g                  z2[i1] = z[i123+mm12] + z[i123];
713.    gG 2 g                  z3[i1] = z[i123+mm1+mm12] + z[i123+mm12] + z1[i1];
714.    gG 2 g---->         }
715.  + gG 2 r4---<         for (i1 = 0; i1 < mm1-1; i1++) {
716.    gG 2 r4               i123 = i1 + mm1*i2 + mm12*i3;
717.    gG 2 r4               j123 = 2*i1 + n1*(2*i2 + n2 * 2*i3);
718.    gG 2 r4                 u[j123] +=  [i123];
719.    gG 2 r4                 u[j123+1] += 0.5*(z[  1]+z[i123]);
720.    gG 2 r4--->         }
```

Loop Accelerated

Loop Partitioned

Loop Not Partitioned

- Loop at line 715 not partitioned
  - Executed redundantly: every thread does every loop iteration

More OpenACC Kernels

- **Insert directive above unpartitioned loop to help compiler:**
  - #pragma acc loop independent
  - (if this didn't work, would use "#pragma acc loop vector" instead)

	Original (Mop/s)	1 kernel (Mop/s)	4 kernels (Mop/s)
Fortran	4787	3509	2727
C	4849	3597	2715 ~~1727~~

- **Fortran and C performance now identical**

Next Steps – Reduce Data Movement

- Need to introduce data regions higher up calltree
- For this, need all callee routines to be accelerated with OpenACC directives
- Use a profiler to map out the calltree to get list of routines
- First need to port some insignificant routines
  - norm2u3, zero3, comm3

Results for Accelerating up the Calltree

- Accelerated loops in norm2u3, zero3, comm3

	Original (Mop/s)	1 kernel (Mop/s)	4 kernels (Mop/s)	Calltree Routines (Mop/s)
Fortran	4787	3509	2727	1884
C	4849	3597	2715	1821

- Slower because even more data movement
  - C still slightly down; poor scheduling, needs acc loop independent

	Original (Mop/s)	1 kernel (Mop/s)	4 kernels (Mop/s)	Calltree Routines (Mop/s)
Fortran	4787	3509	2727	1884
C	4849	3597	2715	1878

Add Data Region

- **Now we put a data region in the main program**
  - Arrays u,v,r are declared create
    - We'll never use the host version of these
  - Arrays a,c are declared copyin
    - They're initialized on the host

- **Then in all the subprograms, we change clauses**
  - Replace copy* and create by present
    - Could replace by present_or_*
      - If we know they should always be present, better to state this
      - Then mistakes become runtime errors rather than just wrong answers
        - We'd have to diagnose these by trawling the runtime commentary

Results with Data Region in Main

- At last, we are running faster (and correctly)!

	Original (Mop/s)	1 kernel (Mop/s)	4 kernels (Mop/s)	Calltree Routines (Mop/s)	Data Region (Mop/s)
Fortran	4787	3509	2727	1884	27583
C	4849	3597	2715	1878	26476

View Compiler Commentary Again

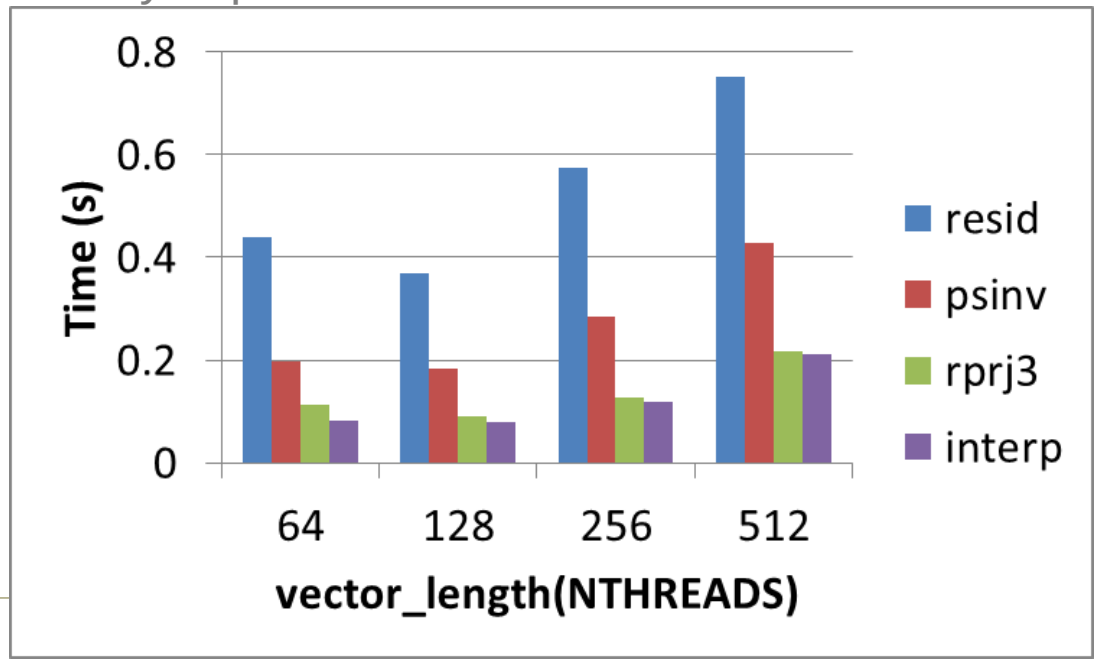
- **All array data transfers eliminated**
  - Run with CRAY_ACC_DEBUG=2 and catch STDERR in a file
  - grep "copy" <file> | sort | uniq

```
ACC:       allocate, copy to acc 'a' (32 bytes)
ACC:       allocate, copy to acc 'c' (32 bytes)
ACC:       allocate, copy to acc 'jg' (320 bytes)
ACC:       allocate reusable, copy to acc <internal> (16 bytes)
ACC:       allocate reusable, copy to acc <internal> (4 bytes)
ACC:       copy to host, done reusable <internal> (16 bytes)
ACC:       reusable acquired, copy to acc <internal> (16 bytes)
```

  - Arrays a, c, jg copied only at initialization
  - Some internal transfers unavoidable

Performance Tuning Tips

- **Check the .lst loopmark file**
  - Are any kernels obviously badly scheduled?
    - No, we already checked that
- **Try varying vector_length from the default of 128**
  - Different values may suit different kernels
  - No effect here: 128 is the best choice
  - Multigrid complicates things;
    - routines called with wide variety of problem sizes



Performance Tuning for resid()

```
DO k = 2,n3-1
 DO j = 2,n2-1
  DO i = 1,n1
   u1(i) = <j,k-stencil on u>
  ENDDO
  DO i = 2,n1-1
   r(i,j,k) = <i-stencil on u1>
  ENDDO
 ENDDO
ENDDO
```

- **Five main tuning options**
  - Loop restructuring
    - Single, perfectly-nested loopnest
      - removing u1 array by manually inlining
      - temporary arrays could be in global memory
    - Two full loopnests
      - explicitly privatised temporaries: u1(i,j,k)
      - perfectly-nested loopnests tend to schedule better
  - Loop scheduling
    - collapse perfectly-nested loops
      - increases flexibility in scheduling loop iterations
    - worker clause on j-loop
      - also increases the amount of parallelism mapped to the accelerator threads
  - Caching re-used data
    - How much: u(i-1:i+1,j,k) or u(i-1:i+1,j-1:j+1,k) or u(i-1:i+1,j-1:j+1,k-1:k+1)
  - Tiling the loopnest
    - especially if we are using the cache clause
  - Varying vector_length (number of threads per block)

So which is best?

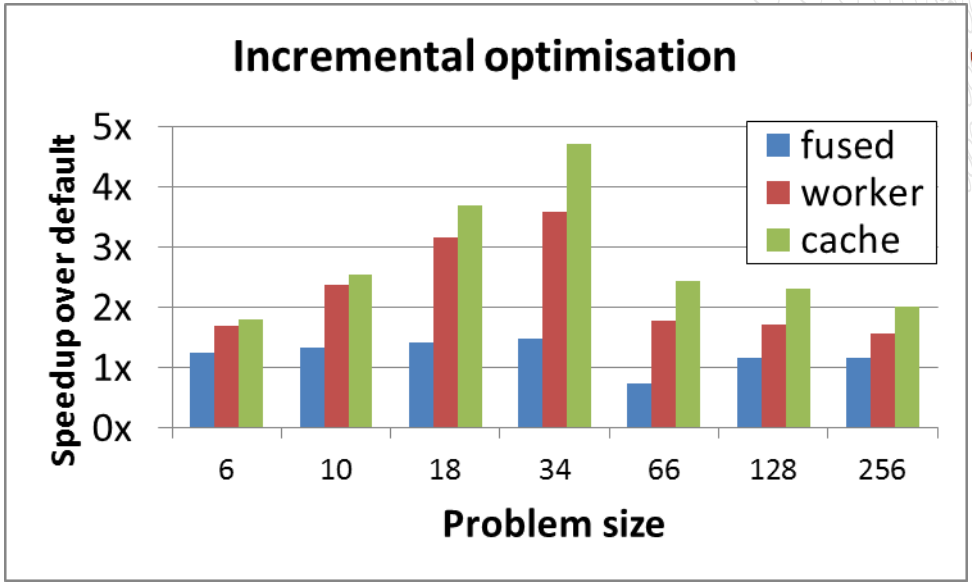
- **Lots of options to explore**
  - best option likely to depend on problem size
    - which varies in a single MG run as we cycle through the blockings
  - may need different algorithm versions for different problem sizes

- **Fortunately, in this case:**
  - best algorithm choice was:
    - single loopnest, worker clause, 1d cache
    - vector_length either 256 or 512 (similar)
    - did not investigate tiling
  - This was best for all problem sizes
    - so we can use same algorithm

```
!$acc parallel loop
DO k = 2,n3-1
!$acc loop worker
 DO j = 2,n2-1
  DO i = 2,n1-1
!$acc cache( u(i-1:i+1,j,k) )
   r(i,j,k) = <full stencil on u>
  ENDDO
 ENDDO
ENDDO
```

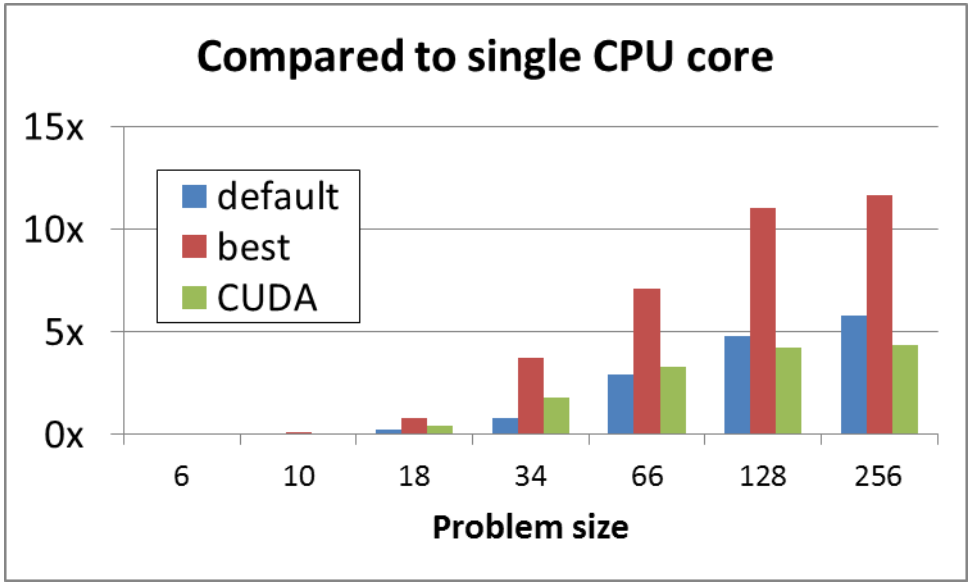
Comparing performance

- **Tuning can work well:**
  - 1.6x to 2.0x gained here
    - depending on problem size



- **OpenACC vs. CPU core:**
  - GPU wins for larger problems
    - default: for 34 and larger
    - tuned: for 18 and larger

- **OpenACC vs. CUDA**
  - even default generally better
  - CUDA here relatively untuned:
    - fused, collapsed, no __shared__
    - but it's much easier to tune OpenACC



Other Performance Tuning Improvements

- **Avoiding temporary arrays in resid:**
  - benefit v. small
  - was it really worth hacking the source?

- **Call an external CUDA version of resid**
  - First attempt (no use of __shared__) is slower
  - This was a naive kernel (there is a lesson in this...)

	Original (Mop/s)	Data Region (Mop/s)	Code change (Mop/s)	CUDA kernel (Mop/s)
Fortran	4787	27583	28993	24262
C	4849	26476	30718	23794

- **Optimising data movements is much more important than kernel tuning**

Conclusions: How far did we get?

- **Significant speedup compared to single core:**
  - Mop/s: 4800 → 27000 = **5½x**
- **The real comparison is to a full CPU**
  - run the OpenMP version of the code on the Intel SandyBridge CPU
    - 4 threads optimal: gives 15000 Mop/s
    - maybe MPI version would scale better, but our code here is scalar
- **Final speedup compared to full CPU:1.8x**

Conclusions: How much further could we get?

- **So we are 1.8x faster, socket-for-socket**
  - How much faster could we get (speeds and feeds)
    - Flops and memory b/w around 5x faster than single Intel Sandybridge
- **So why were we not faster?**
  - MultiGrid application cycles through grid sizes
    - sometimes the grid is really small: 4x4x4
    - CrayPAT loop profiling showed us that
  - Small grid sizes will never schedule well on the GPU
    - consider checking grid size and using different OpenACC for different sizes
    - or do we even need the smaller grids?

OpenACC 4: handling asynchronicity

Exploiting overlap

- **If individual kernels are performing well**
  - Can you start overlapping different computational tasks?
    - kernels on the GPU
    - data transfers to/from the GPU
    - maybe even separate computation on the CPU
- **You can do this using the async features of OpenACC**
  - very similar to streams in CUDA

Asynchronicity

- **GPU operations are launched asynchronously from CPU**
  - control returns immediately to the host
  - host must then wait or test for completion
    - automatically (e.g. handled by OpenACC compiler)
    - manually (e.g. via OpenACC directives or API calls)
  - applies to:
    - computational kernels: parallel and kernels regions
    - PCIe data transfers: update directives
    - plus some other directives

Automatic synchronisation

- **By default, the compiler will handle synchronisation**
  - may be conservative:
    - and wait for every operation to complete
  - may be smarter,
    - and use a reduced number of waits consistent with correctness

- **CCE-specific options:**
  - control with compiler option -hacc_model=auto_async_*
    - auto_async_none :
      - waits for every operation to separately complete
      - useful for debugging and generating profiles
      - but it may skew performance
    - auto_async_kernels :
      - may allow some computational kernels to overlap
      - the default behaviour
    - auto_async_all :
      - may allow kernels and data transfers to overlap
      - try this as a performance-tuning option

User control via async clause

- **The async clause overrides the default behaviour**
  - User is now in control of synchronisation
    - applies to: parallel, kernels, update directives
  - User needs to insert appropriate synchronisation points
    - via wait directive or OpenACC API calls
    - Beware: there is no implicit wait at the end of a subprogram!

- **Between synchronisation points**
  - May get overlap of concurrently-executing kernels
    - depending on hardware
  - Should get overlap of computational kernels with data transfers
    - in both directions on PCIe bus
  - Data transfers in the same direction will not overlap
    - the runtime will automatically serialise the transfers

- **Queuing async operations in advance is a good idea**
  - even if the operations themselves are serialising, get better throughput

A stream of tasks

- **The async clause can take a handle:**
  - async(handle) where handle is a (positive or zero) integer
- **Operations launched with the same handle**
  - guaranteed to execute sequentially in the order they were launched
  - not guaranteed to execute immediately after each other
    - there could be delays
  - this is known as a "stream" of tasks
- **Synchronisation**
  - wait(handle) directive ensures just this stream of tasks has completed
  - can use an API call to do same thing
    - another API call can be used to test whether stream has completed
- **Note**
  - If you've used CUDA streams, these concepts should be very familiar

Multiple streams of tasks

- **You can launch multiple streams of tasks at once**
  - each with a different handle value
  - Tasks within a given stream
    - guaranteed to execute sequentially
  - Tasks in different streams
    - may overlap or serialise, as the hardware and runtime allows
    - operations in different streams should be independent
      - or we have a race condition

- **Synchronisation**
  - wait(handle) directive ensures one stream has completed
    - wait(handle1,handle2,...) can be used to finalise multiple streams
    - wait directive with no argument ensures all streams have completed
  - API calls can be used to wait on, or test for, all these completion cases

- **Nvidia GPUs (Kepler, Fermi)**
  - currently support up to 16 simultaneous streams in hardware
  - if handle is too large, runtime MODs it back into allowable range
    - so handle=16 same as handle=0
    - this can lead to false dependencies between streams

OpenACC async first example

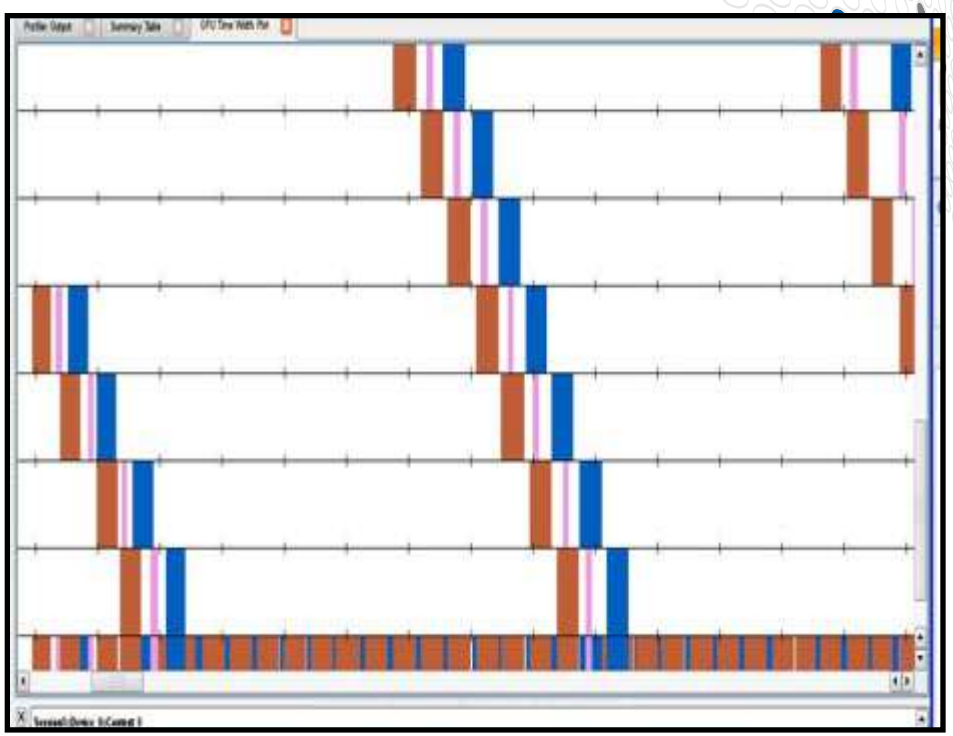
- **a simple pipeline:**
  - processes an array, slice by slice
  - each slice requires 3 tasks:
    - copy data to GPU,
    - process on GPU,
    - bring back to CPU
  - which must execute sequentially
  - but we can overlap different slices

```
REAL :: a(Nvec,Nchunk),b(Nvec,Nchunk)

!$acc data create(a,b)
DO j = 1,Nchunks
!$acc update device(a(:,j)) async(j)

!$acc parallel loop async(j)
  DO i = 1,Nvec
    b(i,j) = <function of a(i,j)>
  ENDDO

!$acc update host(b(:,j)) async(j)

ENDDO
!$acc wait
!$acc end data
```

  - Use a different stream for each slice
    - use slice number as stream handle
    - don't worry if number gets too large
    - OpenACC runtime maps it back into allowable range (using MOD function)

- **Expect to see overlap of three streams at once**
  - one sending to the device; one processing the slice; one sending to host

OpenACC async results



- **Execution times:**
  - CPU: 3.76s
  - OpenACC: 1.10s
  - OpenACC, async: 0.34s
- **NVIDIA Visual profiler:**
  - time flows left to right
  - streams stacked vertically
    - only 7 of 16 streams fit in window
    - **red**: data transfer to device
    - **pink**: computational on device
    - **blue**: data transfer to host
  - vertical slice shows what is overlapping
    - collapsed view at bottom
  - async handle modded by number of streams
    - so see multiple coloured bars per stream (looking horizontally)
- **Alternative to pipelining is task-based overlap**
  - Harder to arrange; needs knowledge of data flow in specific application
  - May (probably will) require application restructuring (maybe helps CPU)

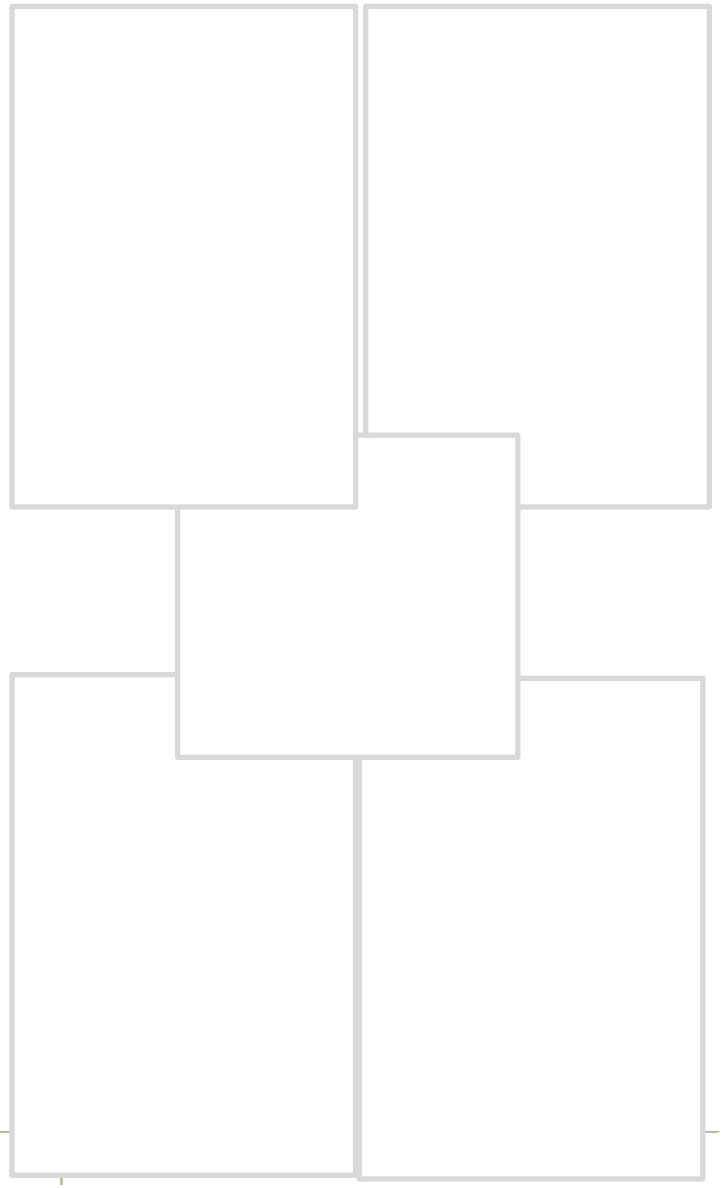
Going further with OpenACC 2.0

- **OpenACC 1.0:**
  - async/wait perfect for handling linear streams of dependent tasks
  - but no way to set up more complicated dependency tree
    - e.g. to say:
      - "When you have finished these streams of tasks, start this one"
      - "When you have finished this stream of tasks, start these ones"
  - dependencies like this have to be handled by the host
    - which means extra host-side synchronisation points, which:
      - reduce the performance of the code
      - reduce developer's ability to use CPU for other tasks in the code

- **OpenACC 2.0:**
  - now allows you to set up dependency tree
  - wait(handle) clause for parallel, kernels, update directives
  - async(handle) clause for wait directive

High-level example

```
!$acc parallel loop async(stream1)
<Kernel A>
!$acc parallel loop async(stream1)
<Kernel B>

!$acc parallel loop async(stream2)
<Kernel C>

!$acc parallel loop async(stream3) &
!$acc     wait(stream1,stream2)
<Kernel D>

!$acc parallel loop async(stream4) &
!$acc     wait(stream3)
<Kernel E>

!$acc parallel loop async(stream5) &
!$acc     wait(stream3)
<Kernel F>

!$acc parallel loop async(stream5)
<Kernel G>

!$acc wait ! ensures all completed
```



Using dependency trees

- **The compiler may use some async automatically**
- **But if you want more control, such as:**
  - multiple, overlapping streams of tasks
  - and, potentially, a more complicated dependency tree
- **Then you will need to do it yourself**
  - This requires:
    - good knowledge of your code (so you know what it does, and where)
    - good knowledge of the algorithm (so you can change the code)
    - good knowledge of the science (so you can change the algorithm)
  - OpenACC improves productivity, but cannot replace the "hard thinking"
- **We'll show a real-world example next**
  - see the parallel Himeno code lecture

OpenACC case study: Porting a parallel code

Alistair Hart
Cray Exascale Research Initiative Europe

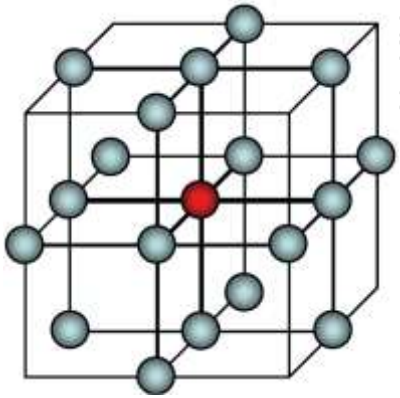
Overview

- **A parallel code is a scalar code with data transfers**
  - We have looked at how to port a scalar code
    - optimising the scalar part procedes in the same way
    - although the local problem size will change when strong scaling
  - Here we look at the parallel version of the same code
- **The new feature is the data transfer between PEs**
  - which also means local data transfers between CPU and GPU
- **This talk looks at the extra things we need to consider**
  - First at a conceptual level
    - the OpenACC part
  - Then some specific points for particular communication models
    - we just discuss MPI here
    - (we also have a version using Fortran coarrays)

Contents

- **Himeno benchmark**
  - Structure of the parallel code
- **Packing and transferring halo buffers**
  - async clause
  - wait clause
- **MPI communication**
  - non-blocking sends and receives
  - MPI_WAITANY vs. MPI_WAITALL
  - G2G optimisations

The Himeno Benchmark



- **Parallel 3D Poisson equation solver**
  - Iterative loop evaluating 19-point stencil
  - Memory intensive, memory bandwidth bound
- **Fortran, C, MPI and OpenMP implementations available from http://accc.riken.jp/2444.htm**
  - Cray also has a Fortran coarray (CAF) version
- **Productivity of OpenACC**
  - ~600 lines of Fortran
  - Fully ported to accelerator using around 30 directive pairs

Overall program structure

- **Like scalar case:**
  - initmt() initialises data
  - jacobi(nn,gosa)
    - does nn iterations
    - stencil update to data
  - called twice:
    - once for calibration
    - once for measurement
- **differences:**
  - initcomm() routine
    - sets up processor grid

```
PROGRAM himeno
   CALL initcomm    ! Set up processor grid
   CALL initmt      ! Initialise local matrices

   cpu0 = gettime() ! Wraps SYSTEM_CLOCK
   CALL jacobi(3,gosa)
   cpu1 = gettime()
   cpu = cpu1 - cpu0

!  nn = INT(ttarget/(cpu/3.0)) ! Fixed runtime
   nn = 1000        ! Hardwired for testing

   cpu0 = gettime()
   CALL jacobi(nn,gosa)
   cpu1 = gettime()
   cpu = cpu1 - cpu0

   xmflops2 = flop*1.0d-6/cpu*nn

   PRINT *,' Loop executed ',nn,' times'
   PRINT *,' Gosa :',gosa
   PRINT *,' MFLOPS:',xmflops2,'  time(s):',cpu
END PROGRAM himeno
```

The distributed jacobi routine

- iteration loop:
  - fixed tripcount
- jacobi stencil:
  - temporary array **wrk2**
  - local residual **wgosa**
- halo exchange
  - between neighbours
  - uses send, receive buffers
- Residual
  - global residual **gosa**
  - **wgosa** summed over PEs
- second kernel:
  - **p** updated from **wrk2**

```
iter_lp: DO loop = 1,nn

  compute stencil: wrk2, wgosa from p

  pack halos from wrk2 into send bufs

  exchange halos with neighbour PEs

  sum wgosa across PEs

  copy back wrk2 into p

  unpack halos into p from recv bufs

ENDDO iter_lp
```

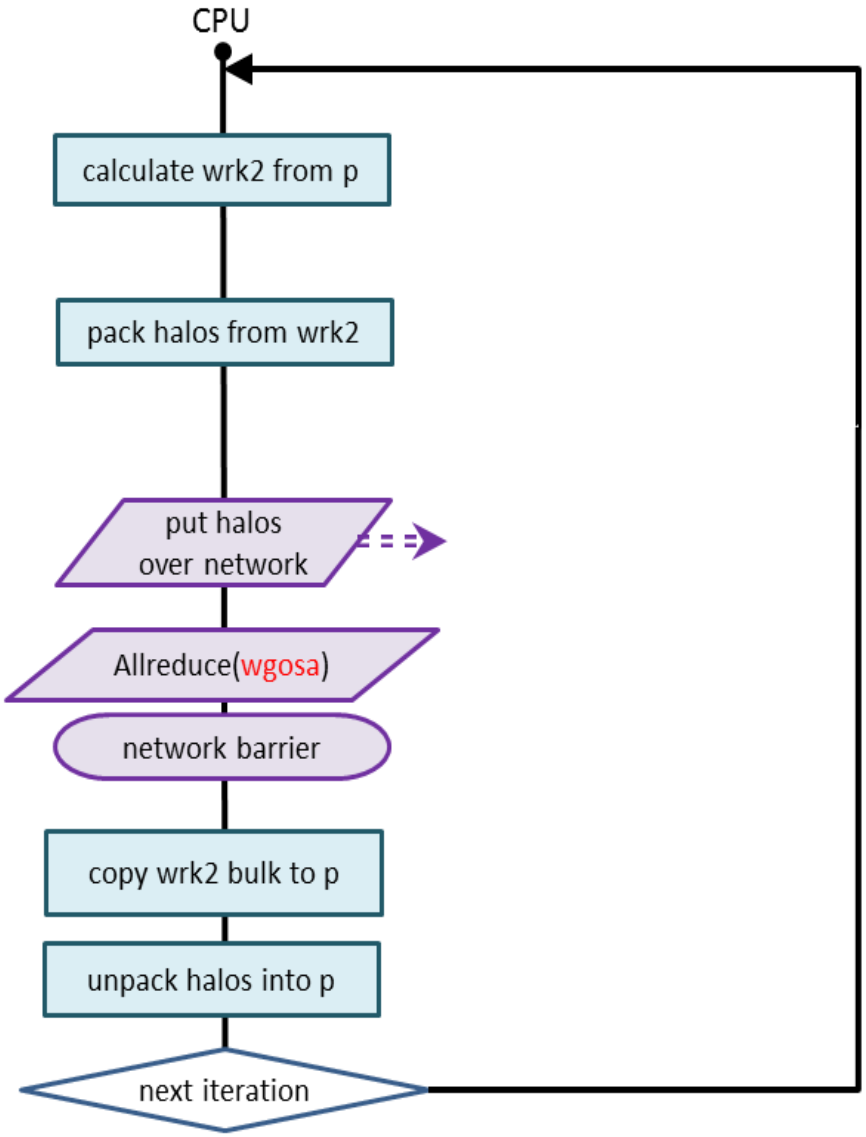
The Jacobi computational kernel (serial)

- The stencil is applied to pressure array **p**
- Updated pressure values are saved to temporary array **wrk2**
- Local control value **wgosa** is computed

```
DO K=2,kmax-1
 DO J=2,jmax-1
  DO I=2,imax-1
   s0=a(I,J,K,1)* p(I+1,J, K )                                    fwd n.n.
     +a(I,J,K,2)* p(I, J+1,K ) &
     +a(I,J,K,3)* p(I, J, K+1) &
     +b(I,J,K,1)*(p(I+1,J+1,K )-p(I+1,J-1,K )  &                  n.n.n.
                  -p(I-1,J+1,K )+p(I-1,J-1,K )) &
     +b(I,J,K,2)*(p(I, J+1,K+1)-p(I, J-1,K+1)  &
                  -p(I, J+1,K-1)+p(I, J-1,K-1)) &
     +b(I,J,K,3)*(p(I+1,J, K+1)-p(I-1,J, K+1)  &
                  -p(I+1,J, K-1)+p(I-1,J, K-1)) &
     +c(I,J,K,1)* p(I-1,J, K ) &                                  bwd n.n.
     +c(I,J,K,2)* p(I, J-1,K ) &
     +c(I,J,K,3)* p(I, J, K-1) &
     + wrk1(I,J,K)

   s = (s0*a(I,J,K,4)-p(I,J,K))*bnd(I,J,K)
   wgosa = wgosa + ss*ss
   wrk2(I,J,K) = p(I,J,K) + omega * ss
  ENDDO
 ENDDO
ENDDO
```

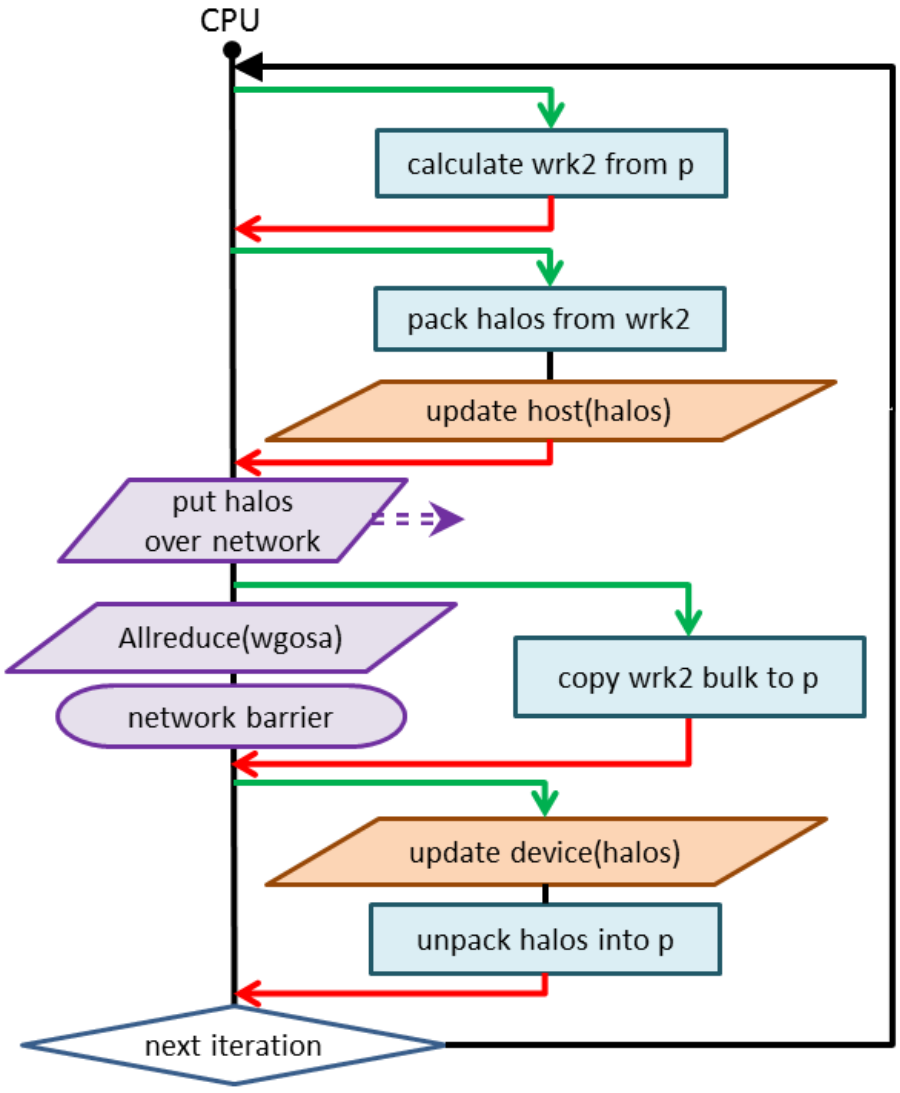
Distributed jacobi routine as a flowchart

- take advantage of overlap
  - just network at this point
- still some freedom:
  - barrier can move relative to
    - Allreduce
    - wrk2→bulk
- Which is best order?
  - depends on:
    - hardware
    - comms library
    - kernel details
    - local problem size
  - Could autotune this
    - separately
    - at runtime



First OpenACC port

- **Loopnest kernels**
  - stencil
  - pack halos: x, y, z
  - wrk2→bulk
  - unpack halos: x, y, z
- **acc updates**
  - 6 buffers each time
- **Some additional overlap**
  - GPU kernels asynchronous
  - wrk2→bulk
    - can overlap with comms



Packing and transferring send buffers

- **Use async clause**
  - separate handles for overlap
    - one per direction
      - three in total
      - integers, e.g. 1, 2, 3
  - what about six streams?
    - one each for up and down
    - was not as efficient
      - but this is a tuning option
  - global wait
    - all 3 streams completed

```
!$acc parallel loop async(xstrm)
DO k = 2,kmax-1
  DO j = 2,jmax-1
    sendbuffx_dn(j,k)=wrk2(2,j,k)
    sendbuffx_up(j,k)=wrk2(imax-1,j,k)
  ENDDO
ENDDO
!$acc end parallel loop

!$acc update host &
!$acc    (sendbuffx_dn,sendbuffx_up) &
!$acc   async(xstrm)

! same for y with async(ystrm)
! same for z with async(zstrm)

!$acc wait
<send the 6 buffers>
```

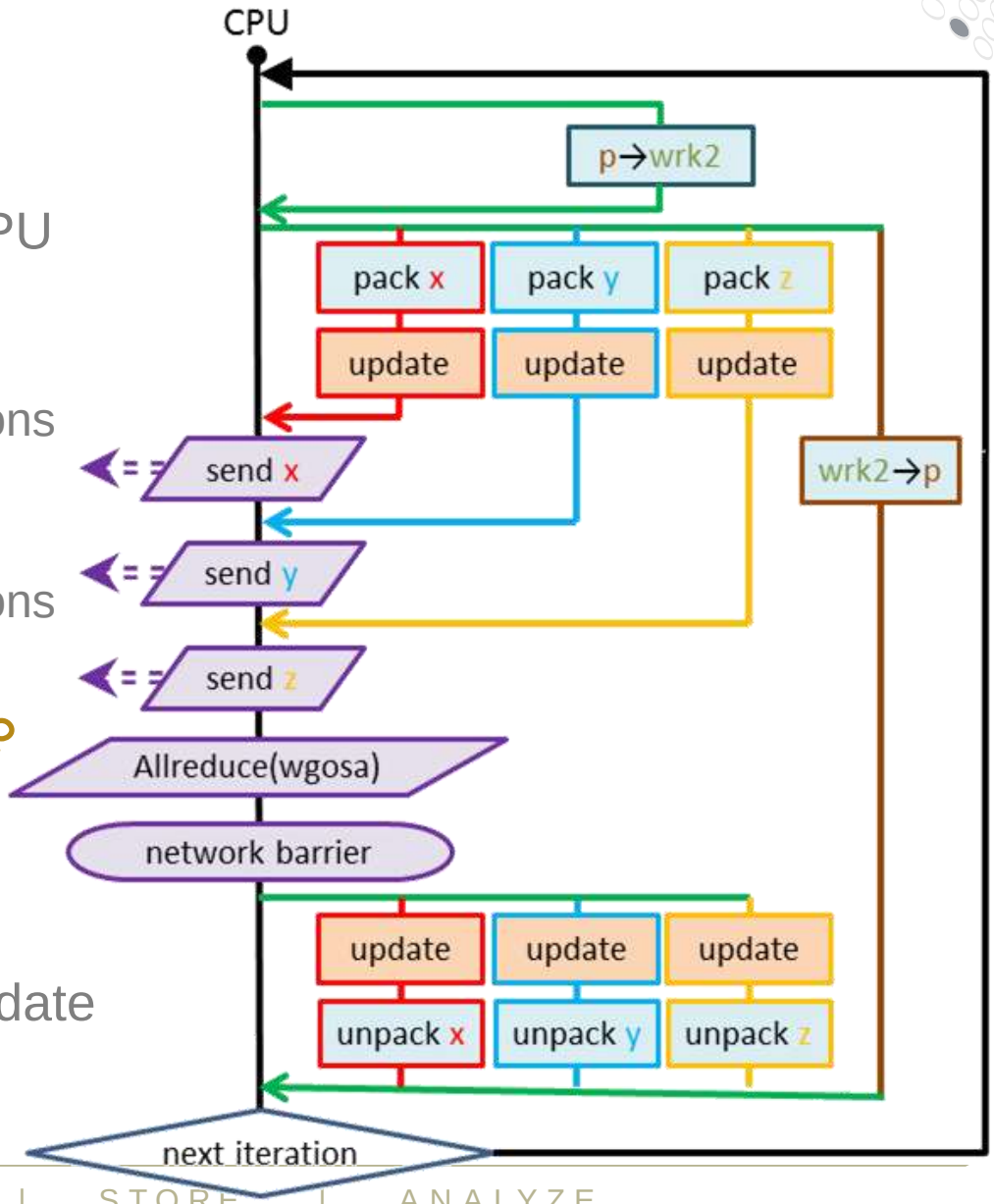
Packing and transferring send buffers (better)

- **The biggest bottleneck**
  - PCIe link serialises:
    - only one buffer moves at a time
  - A better strategy:
    - don't wait for all to finish moving
    - as soon as one direction done
    - send these buffers over network
  - Ordering:
    - x pack/update starts first
    - Can we guarantee x ready first?
    - No, but it is likely
  - No OpenACC "waitany" facility
    - so we go with most likely ordering

```
!$acc parallel loop async(xstrm)
<pack the two x buffers>
!$acc end parallel loop

!$acc update host &
!$acc (sendbuffx_dn,sendbuffx_up) &
!$acc  async(xstrm)

! same for y with async(ystrm)
! same for z with async(zstrm)

!$acc wait(xstrm)
<send the two x buffers>

!$acc wait(ystrm)
<send the two y buffers>

!$acc wait(zstrm)
<send the two z buffers>
```

Graphically

- **async clause**
  - allows task overlap on GPU
  - halo pack/update
    - can overlap x, y, z directions
  - halo update/unpack
    - can overlap x, y, z directions
  - can also overlap **`wrk2→p`**
- **Host/GPU sync points**
  - After first kernel
  - After each buffer pack/update
  - At the end of the iteration



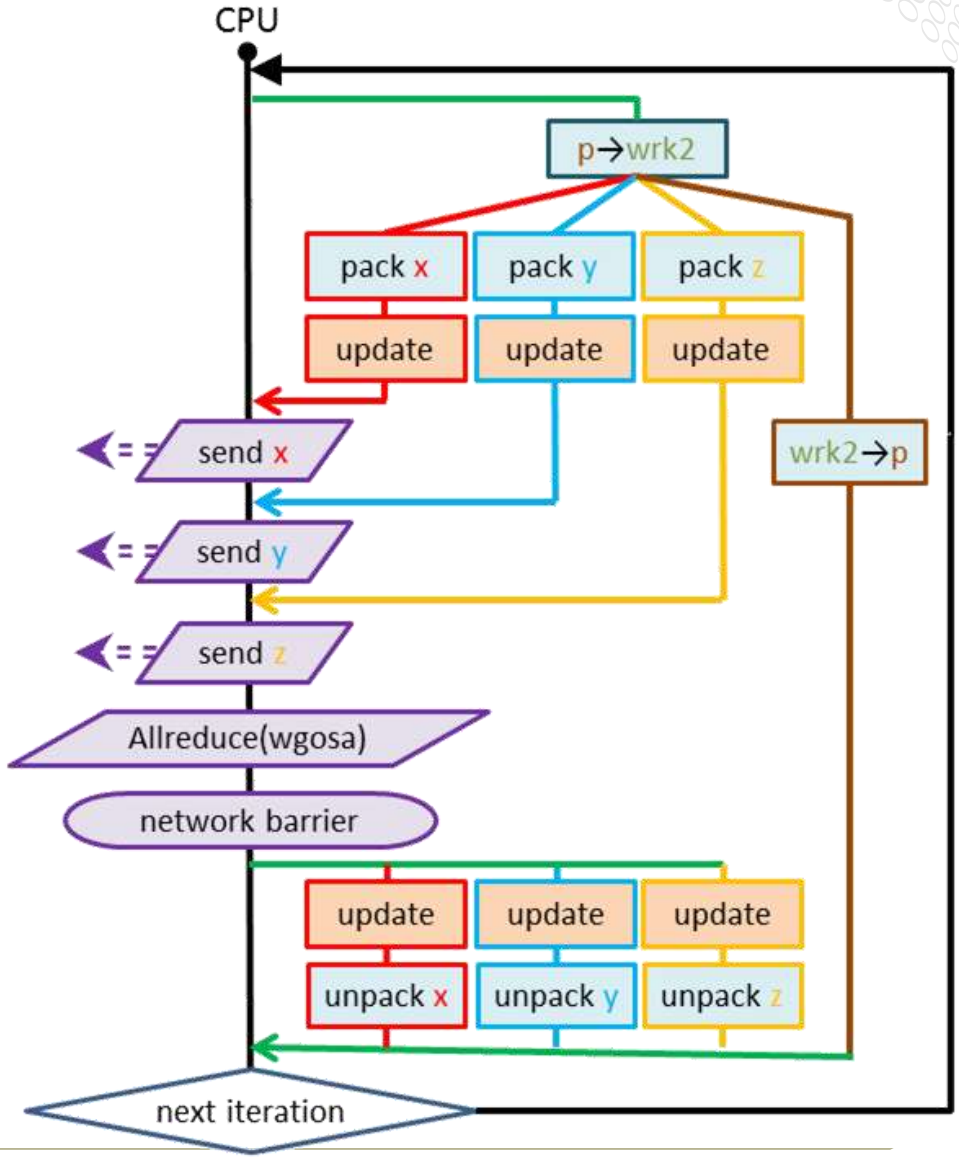
Transferring and unpacking recv buffers

- **Copying `wrk2` into `p`**
  - very quick kernel
  - but can overlap with network
    - could start this kernel before we sent the data
- **When messages complete**
  - copy and unpack recv buffers
  - three parallel streams again
- **wait**
  - ensures all 4 streams complete
    - 3 update/unpacks plus bulk
  - ready to start next iteration

```
!$acc parallel loop async(bstrm)
<copy bulk wrk2 -> p>
!$acc end parallel loop

<network barrier>

!$acc update device &
!$acc  (recvbuffx_dn,recvbuffx_up) &
!$acc  async(xstrm)

!$acc parallel loop async(xstrm)
<unpack the two x buffers>
!$acc end parallel loop

! same for y with async(ystrm)
! same for z with async(zstrm)

!$acc wait

<end iteration loop>
```

Using the OpenACC v2.0 wait clause

- **Launch 5 operations**
  - stencil kernel
  - 3 buffer packs/updates
    - depends on stencil kernel
  - 1 bulk unpack
    - also depends on stencil
- **wait clause**
  - sorts out dependencies
- **host/device sync points**
  - no longer need after initial, stencil kernel



Using the OpenACC v2.0 wait clause

- **In more detail:**
- **Introduce new stream**
  - jstrm for stencil kernel
  - buffer-packing streams wait on this completing
  - acc wait(xstrm) guarantees jstrm has also completed
    - (also waits on ystrm, zstrm)
- **bulk copy kernel also waits on jstrm**
  - we don't set jstrm=bstrm
  - want to kick-off buffer packs as soon as **wrk2** is ready

```
!$acc parallel loop async(jstrm)
<stencil p -> wrk2>

!$acc parallel loop &
!$acc   async(xstrm) wait(jstrm)
<pack x buffers from wrk2>

!$acc update host &
!$acc   (sendbuffx_dn,sendbuffx_up) &
!$acc   async(xstrm)

! same for y with async(ystrm)
! same for z with async(zstrm)

!$acc parallel loop &
!$acc   async(bstrm) wait(jstrm)
<copy bulk wrk2 -> p>

!$acc wait(xstrm)
<send the two x buffers>

! same for y with async(ystrm)
! same for z with async(zstrm)
```

Data region considerations

- **Twelve extra buffers needed**
  - 3 physical dimensions: x, y, z
    - 2 directions of transfer: up, down
      - 2 separate buffers: send, receive

- **These buffers need to be added to the data region(s)**
  - if just in jacobi() data region
    - they should be create
      - allocated each time jacobi() is called, no data transfer (except explicit updates)
  - or in outer data region
    - create in main data region
    - present in jacobi() data region
    - need to be declared globally
  - *advice:*
    - *if jacobi() routine is called a lot, often better to allocate once in parent*

MPI

- **Use nonblocking MPI calls**
  - MPI_IRECV
    - post these receives early; first thing in iteration loop
  - MPI_ISEND
    - call these in 3 sets (x, y, z) of two (up, down)
      - after each of async streams xstrm, ystrm, zstrm separately completes
  - network barrier:
    - MPI_WAITALL(12,send_recv_handles(:))
    - ensures all buffers arrive (and send buffers can be reused)
  - Then kick-off the three streams copying recv buffers to accelerator and unpacking

Better host-side MPI

- **PCIe transfer of three sets of recv buffers is a bottleneck**
  - buffer transfers will serialise, one at once
  - better to start transfer of messages to GPU as soon as each arrives
    - don't know in which order the 6 message will arrive
- **Rather than MPI_WAITALL(12,send_recv_handles(:))**
  - Loop over MPI_WAITANY(6,recv_handles(:))
    - As each arrives, start separate async stream comprising:
      - update, then unpack kernel
    - 6 different streams being used here
- **After all MPI recvs completed:**
  - MPI_WAITALL(6, send_handles(:))
    - so we the send buffers are ready for reuse in the next iteration
  - acc wait ensures 7 streams have completed
    - 6 copy/unpacks, plus the bulk stream
- **Could also use MPI3 nonblocking collective for gosa**
  - would MPI_WAIT on this handle just before end of iteration loop

Improved G2G MPI

- **Latest Cray MPICH library offers "G2G" feature**
  - Can call MPI on CPU, but passing GPU buffer to library
  - Data moves between GPU and network seamlessly
    - no need for update directives
    - no need for host-side synchronisation between update and send/recv
      - when MPI completes, know data has moved
      - fewer sync points allows more flexible overlap of CPU and GPU operations
    - improved end-to-end communication bandwidth
- **host_data directive used to expose device data pointers**
  - Put host_data regions around MPI calls
- **Code can still be compiled for the CPU**

Using the G2G MPI

- **Receives**
  - posted with GPU buffers
- **updates removed**
  - just pack buffers on GPU
- **Sends**
  - also use GPU addresses
- **MPI_WAITALL**
  - data now moved to recv buffers on remote GPUs
  - no extra GPU sync needed
  - no need for MPI_WAITANY any more
    - can use 3 unpack streams

```
!$acc host_data use_device &
        (recvbuffx_dn,recvbuffx_up)
call MPI_IRECV(recvbuffx_dn,...)
call MPI_IRECV(recvbuffx_up,...)
!$acc end host_data
! same for y,z

<stencil p -> wrk2> async(jstrm)

<pack x buffs> async(xstrm) wait(jstrm)
! same for y,z

!$acc wait(xstrm)
!$acc host_data use_device &
        (sendbuffx_dn,sendbuffx_up)
call MPI_ISEND(sendbuffx_dn,...)
call MPI_ISEND(sendbuffx_up,...)
!$acc end host_data
! same for y,z

call MPI_WAITALL(12,...)

<unpack x buffs> async(xstrm)
! same for y,z

!$acc wait
```

Summary

- **A parallel code is just like a scalar code**
- **but with data transfers**
  - These data transfers add additional complications
  - Provide a lot of scope for overlap:
    - overlapping GPU kernels/transfers
    - overlapping compute and network transfers
  - A lot of scope implies a lot of algorithmic choices
    - Which is best will depend on the code, the problem, the parallel decomposition and the hardware
    - An autotuning approach may help
- **General advice:**
  - Profile the production code frequently and optimise the slowest bit
    - Could be kernel performance or network transfers
    - The balance will shift as you continue optimising

Summary

- **Some things to look for**
  - look for opportunities to overlap GPU tasks with the async clause
    - e.g. packing buffers in different directions
  - look for opportunities to exploit the wait clause
    - going beyond simple streams of tasks to a dependency tree
  - use asynchronous MPI
    - if you are not already doing so
    - extra PCIe transfer time gives more scope for network overlap
  - try MPI_WAITANY rather than MPI_WAITALL
    - to exploit this potential for extra overlap
  - or use G2G MPI to remove host-side synchronisation points
    - and improve data transfer rates between accelerators on different nodes
- **The same principles apply more widely**
  - to other message-passing programming models
  - CAF, SHMEM etc.

OpenMP and OpenACC a Comparison

Outline

- **Background**
  - OpenMP
  - OpenACC
- **Important differences (today)**
  - Parallelism
  - Present_or_*
  - Scalars
  - Loops
  - Unstructured data
  - Calls (separate compilation units)
  - Nested parallelism
- **What is next**
  - OpenMP
  - OpenACC

Background -- OpenMP

- FORTRAN version 1.0 - (October 1997)
- Accelerator additions
  - Proposal submitted Dec 2009
  - Subcommittee formed Aug 2009
- Cray OpenMP for Accelerators nears release
- Fall 2010 several members for OpenACC working group
- TR1 - Technical Report on Directives for Attached Accelerators (November 2012)
- OpenMP 4.0 (July 2013)

Background -- OpenACC

- PGI releases accelerator directives
- CAPS releases HMPP
- Fall 2010 several members form OpenACC working group
- OpenACC 1.0 (Nov 2010)
- OpenACC 2.0 (June 2013)

Important differences

- Parallelism
- Present_or_*
- Scalars
- Loops
- Calls (separate compilation units)

Parallelism

- **OpenACC**
  - "Off-load" and parallel startup tied together
    - Acc parallel
    - Acc kernels
- **OpenMP**
  - "Off-load" and parallel startup disconnected
    - Omp target
      - Omp parallel
      - Omp teams

Parallel startup example (Fortran)

OpenACC

```
!$acc parallel
…
!$acc end parallel
```

Or

```
!$acc kernels
…
!$acc end kernels
```

OpenMP

```
!$omp target
!$omp teams/parallel
…
!$omp end teams
!$omp end target
```

Parallel startup example (C/C++)

OpenACC

```
#pragma acc parallel
{
…
}
```

Or

```
#pragma acc kernels
{
…
}
```

OpenMP

```
#pragma omp target
#pragma omp teams/parallel
{
…
}
```

OpenMP teams vs parallel

- **Why two different "parallel" mechanisms**
- **Teams**
  - Independent collision domains
  - Same behavior as OpenACC gangs
  - Only select directives allowed
- **Parallel**
  - A single collision domain
  - Default if neither is present
  - All non-accelerator OpenMP directives allowed

Present_or_*

- **OpenACC**
  - present_or_* programmer visible
    - copy, copyin, copyout, create
  - copy* without present allowed
    - Error prone
    - Hard to debug
    - Little actual savings
- **OpenMP**
  - present_or_* not programmer visible
  - map always implies present test
    - in, out, inout, allocate

Scalars

- **OpenACC**
  - firstprivate by default
  - User can override
    - Error prone
  - Allows implementation to make these kernels arguments
  - Pointers are “special”

- **OpenMP**
  - No such restriction
  - Pointers are scalars

Loops

- **OpenACC**
  - One construct “loop”
  - Multiple parallelism types
  - “nested” parallelism implicit
  - Three levels available
    - gang
    - worker
    - vector
- **OpenMP**
  - Three constructs
    - distribute
    - do/for
    - simd
  - Nested parallelism explicit

Loop examples

OpenACC

```
!$acc loop
do i=1,n
…
enddo
```

OpenMP

```
!$omp do
or
!$omp distribute
do i=1,n
…
enddo
!$omp end distribute
or
!$omp end do
```

Loop examples

OpenACC

```
!$acc loop
do i=1,n
!$acc loop
  do j=1,m
   …
  enddo
enddo
```

OpenMP

```
!$omp distribute
do i=1,n
!$omp parallel do
  do j = 1,m
   …
  enddo
!$omp end parallel do
enddo
!$omp end distribute
```

Loop examples

OpenACC

```
!$acc loop gang worker vector
do i=1,n
…
enddo
```

OpenMP

```
!$omp distribute parallel do simd
do i=1,n
…
enddo
!$omp end distribute parallel do simd
```

Unstructured data

- **Separate the move to and the move from parts of data constructs**
- **enter data**
  - constructors
- **exit data**
  - destructors
- **OpenACC**
  - Added support in 2.0
- **OpenMP**
  - Nearing completion of feature

Calls

- **OpenACC**
  - routine
  - Only one type of parallelism allowed
    - gang
    - worker
    - vector
    - seq
  - Hard on user
  - Easy for implementer
- **OpenMP**
  - declare
    - Type of parallelism ignored
  - Easy on user
  - Hard for implementer

Nested parallelism

- **OpenACC**
  - Added in 2.0
  - Currently no full implementations
    - Why?

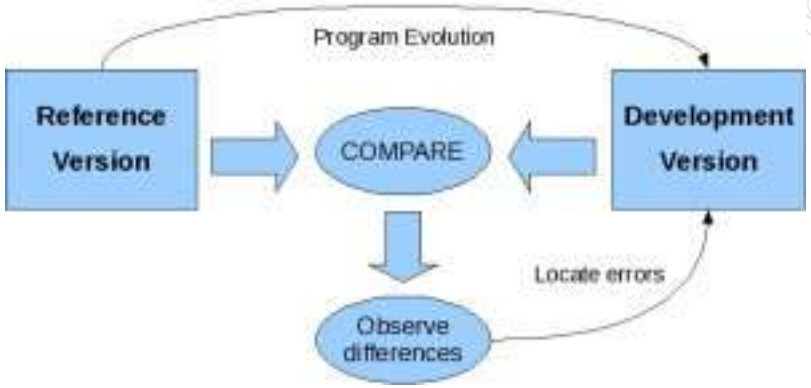
- **OpenMP**
  - parallel inside of teams is allowed
  - teams inside of teams is not allowed.

What is next

- **OpenACC**
  - Tools interfaces
  - Better user defined type support
  - …
- **OpenMP**
  - What is next
  - Unstructured data
  - Declare target deferred_map
  - Interoperability with accelerated libraries
  - Multiple devices
  - User defined type support

Cray Comparative Debugger (CCDB)

- **What is comparative debugging?**
  - Data centric approach
  - Two applications, same data
  - Key idea: The data should match
  - Quickly isolate deviating variables

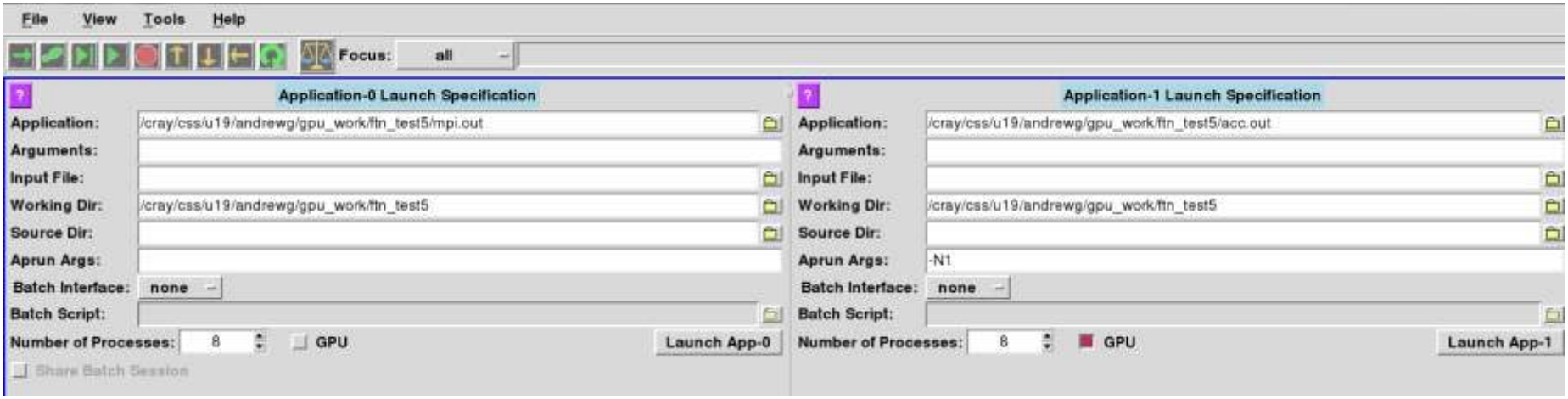


- **CCDB**
  - NOT a traditional debugger!
  - Assists with comparative debugging
  - GUI hides the complexity and helps automate process
    - Creates automatic comparisons
    - Based on symbol name and type
    - Allows user to create own comparisons
    - Error and warning epsilon tolerance
    - Scalable

- **How does this help me?**
  - Algorithm re-writes
  - Language ports
  - Different libraries/compilers
  - New architectures

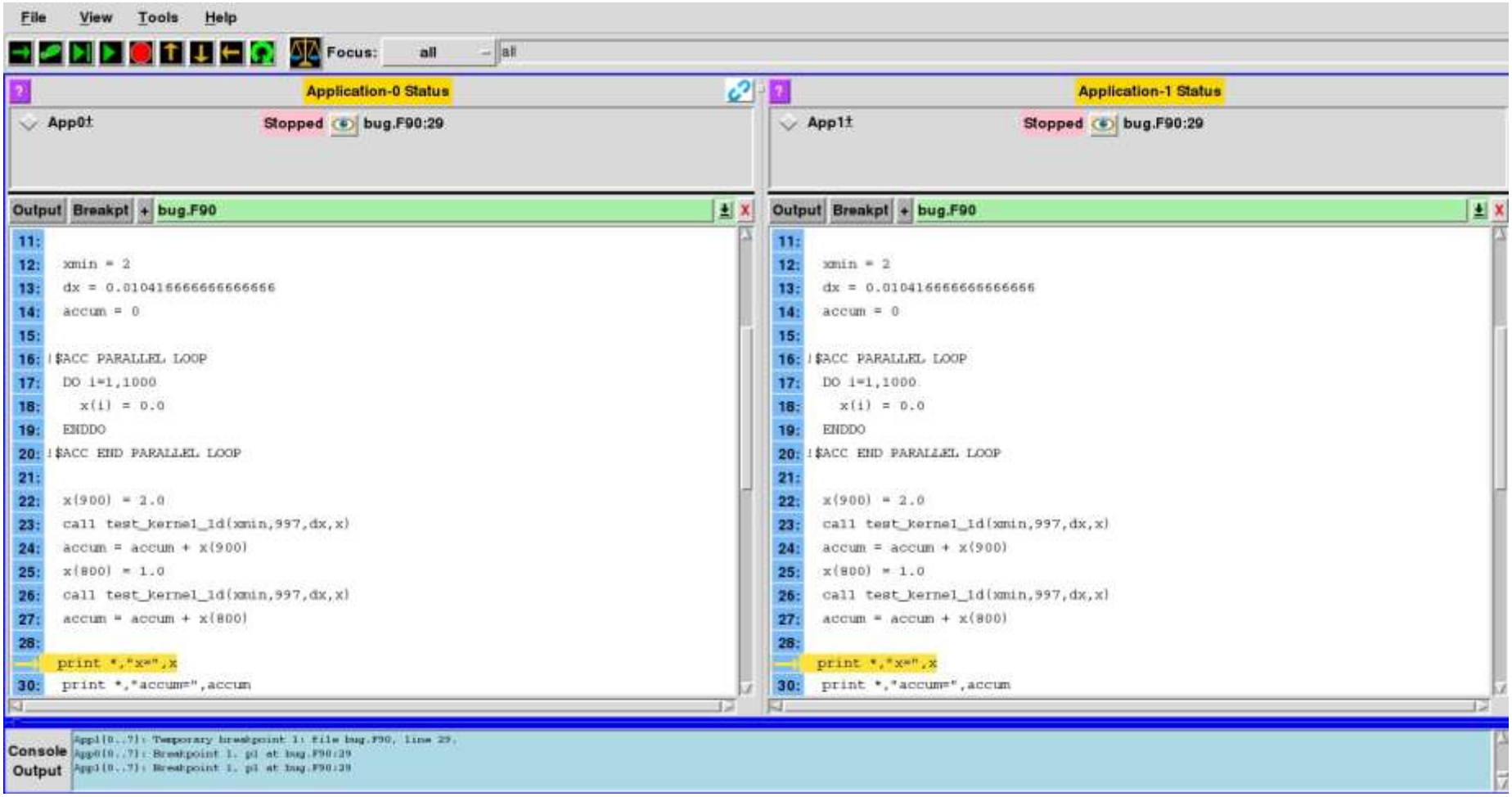
Launching the Applications

- **Reference application**
  - MPI on X86
- **Faulty application**
  - OpenACC on X86 + K20

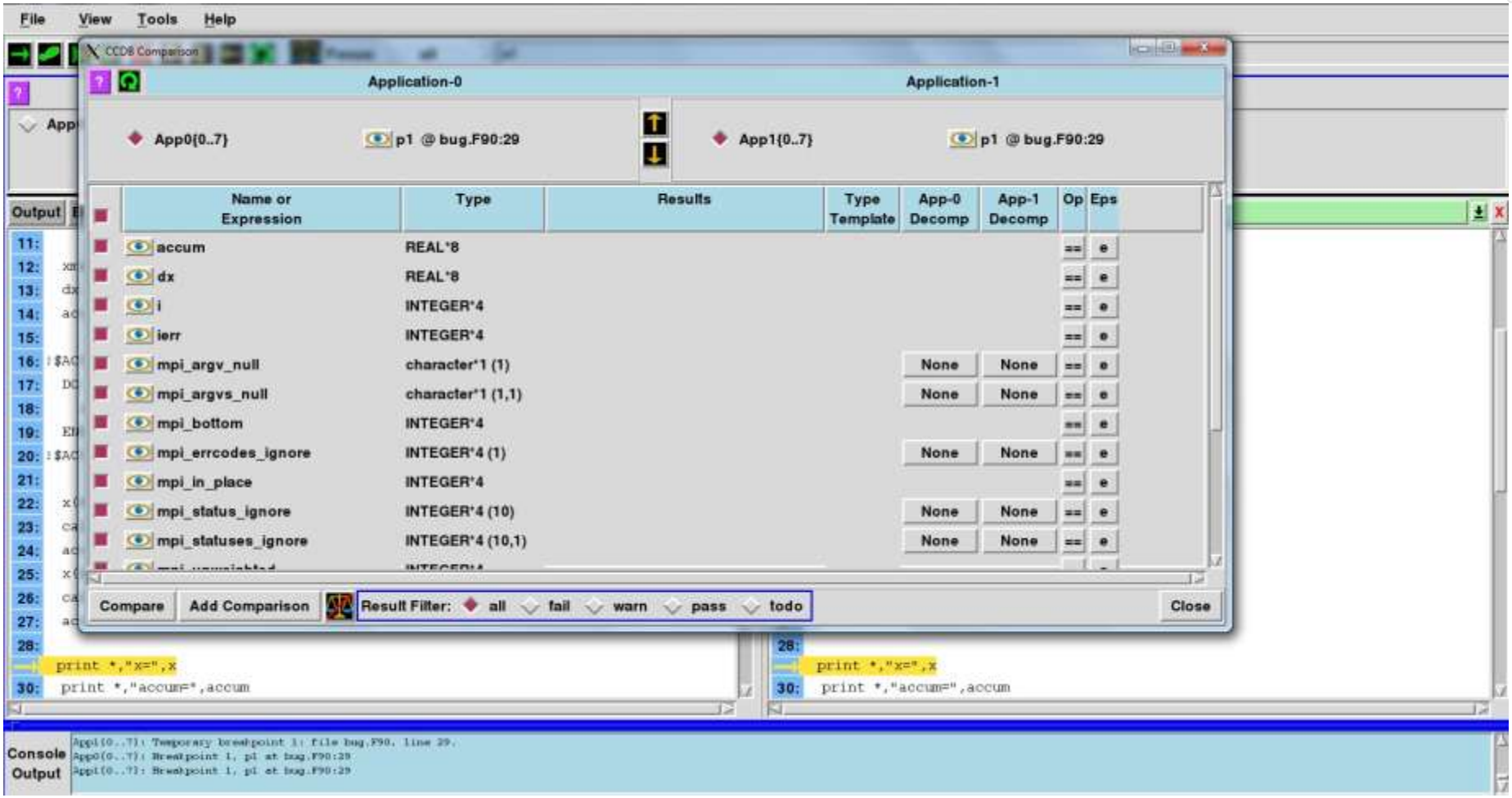


Comparative Debugging from Output

- Setup breakpoint where result is printed



Compare Variables



Verify Failing Comparisons

Go Back to Where Results Agree

Continue to Next Assignment to X

What is in test_kernel_1d?

```
36: SUBROUTINE test_kernel_1d(x_min,x_max,dx,x_dim)
37:   IMPLICIT NONE
38:
39:   INTEGER         :: x_min,x_max
40:   REAL(KIND=8)    :: dx
41:   REAL(KIND=8), DIMENSION(x_min-2:x_max+3) :: x_dim
42:   INTEGER         :: j
43:
44: !$ACC PARALLEL LOOP ASYNC
45:   DO j=x_min-2,x_max+3
46:     x_dim(j) = x_min+dx*float(j-x_min)+x_dim(j)
47:   ENDDO
48: !$ACC END PARALLEL LOOP
49:
50: END SUBROUTINE test_kernel_1d
```

In conclusion

- This has been a brief tutorial introducing OpenACC
- We only covered a part of the standard
- But... you can do a lot of acceleration using just this
- And if you have any questions, please ask!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