



Threaded programming

Introduction to performance optimisation

Slides contributed by Cray and EPCC





Why?

- Large computer simulations are becoming common in many scientific disciplines.
- These often take a significant amount of time to run.
 - Sometimes they take too long.
- There are three things that can be done
 - Change the science (compromise the research)
 - Change the computer (spend more money)
 - Change the program (this is performance optimisation)





What?

- There are usually many different ways you can write a program and still obtain the correct results.
- Some run faster than others.
 - Interactions with the computer hardware.
 - Interactions with other software.
- Performance optimisation is the process of making an existing working computer program run faster in a particular Hardware and Software environment.
 - Converting a sequential program to run in parallel is an example of optimisation under this definition!





When?

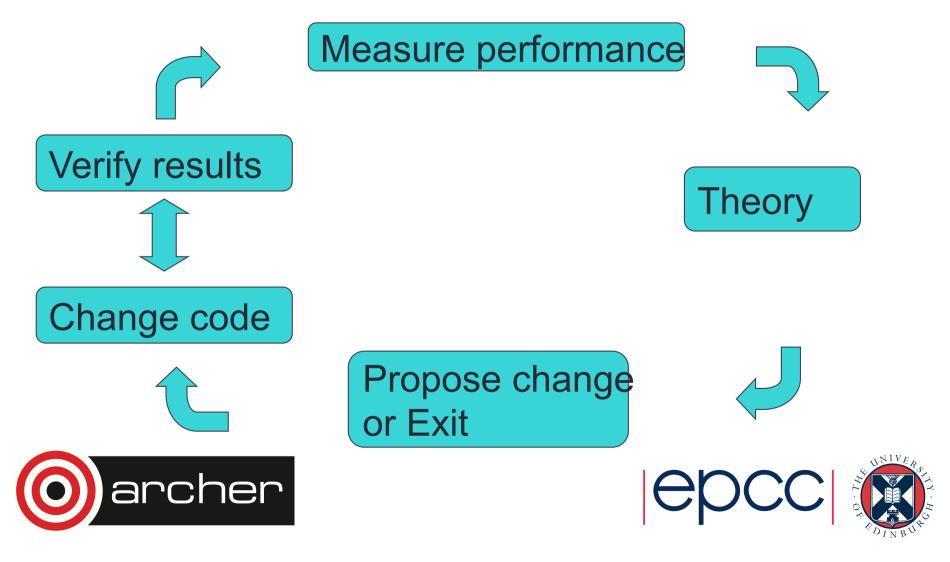
- Performance optimisation can take large amounts of development time.
- Some optimisations improve program speed at the cost of making the program harder to understand (increasing the cost of future changes)
- Some optimisations improve program speed at the cost of making the program more specialised and less general purpose.
- It is always important to evaluate the relative costs and benefits when optimising a program
 - This requires the ability to estimate potential gains in advance





How?

• Performance optimisation usually follows a cycle:



Measuring performance

- It is not enough to just measure overall speed
 - You need to know where the time is going.
- There are tools to help you do this
 - They are called profiling tools.
- They give information about:
 - Which sections of code are taking the time
 - Sometimes line by line but usually only subroutines.
 - Sometimes the type of operation
 - memory access
 - floating point calculations
 - file access
- Make sure you understand how variable your results are
 - Are the results down to my changes or just random variation?





Input dependence

- Many codes perform differently with different input data.
- Use multiple sets of input data when measuring performance.
- Make sure these are representative of the problems where you want the code to run quickly.



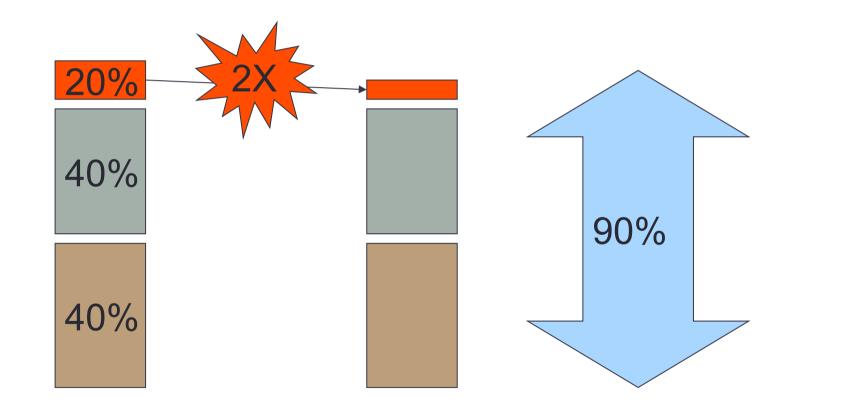


Only optimise important sections

- Its only worth working on parts of the code that take a lot of time.
- Large speed-up of unimportant sections have little impact on the overall picture.
 - Amdahl's law is this concept applied to parallel processing.
 - Same insight applies to other forms of optimisation.











What is profiling?

- Analysing your code to find out the proportion of execution time spent in different routines.
- Essential to know this if we are going to target optimisation.
- No point optimising routines that don't significantly contribute to the overall execution time.
 - can just make your code less readable/maintainable





Code profiling

- Code profiling is the first step for anyone interested in performance optimisation
- Profiling works by instrumenting code at compile time
 - Thus it's (usually) controlled by compiler flags
 - Can reduce performance
- Standard profiles return data on:
 - Number of function calls
 - Amount of time spent in sections of code
- Also tools that will return hardware specific data
 - Cache misses, TLB misses, cache re-use, flop rate, etc...
 - Useful for in-depth performance optimisation





Sampling and tracing

- Many profilers work by sampling the program counter at regular intervals (normally 100 times per second).
 - low overhead, little effect on execution time
- Builds a statistical picture of which routines the code is spending time in.
 - if the run time is too small (< ~10 seconds) there aren't enough samples for good statistics
- Tracing can get more detailed information by recording some data (e.g. time stamp) at entry/exit to functions
 - higher overhead, more effect on runtime
 - unrestrained use can result in huge output files





Standard Unix profilers

- Standard Unix profilers are prof and gprof
- Many other profiling tools use same formats
- Usual compiler flags are -p and -pg:
 - ftn -p mycode.F90 -o myprog for prof
 - cc -pg mycode.c -o myprog for gprof
- When code is run it produces instrumentation log
 - mon.out for prof
 - gmon.out for gprof
- Then run prof/gprof on your executable program
 - eg.gprof myprog (not gprof gmon.out)





Standard profilers

• prof myprog reads mon.out and produces this:

%Time	Seconds	Cumsecs	#Calls	msec/call	Name
32.4	0.71	0.71	14	50.7	relax_
28.3	0.62	1.33	14	44.3	resid_
11.4	0.25	1.58	3	83.	f90_close
5.9	0.13	1.71	1629419	0.0001	_mcount
5.0	0.11	1.82	339044	0.0003	f90_slr_i4
5.0	0.11	1.93	167045	0.0007	
inrange_single					
2.7	0.06	1.99	507	0.12	_read
2.7	0.06	2.05	1	60.	MAIN_





Standard profilers

- **gprof myprog** reads **gmon.out** and produces something very similar
- gprof also produces a program calltree sorted by inclusive times
- Both profilers list all routines, including obscure system ones
 - Of note: mcount(), _mcount(), moncontrol(), _moncontrol() monitor() and _monitor() are all overheads of the profiling implementation itself
 - _mcount() is called every time your code calls a function; if it's high in the profile, it can indicate high function-call overhead
 - gprof assumes calls to a routine from different parents take the same amount of time – may not be true





The Golden Rules of profiling

- Profile your code
 - The compiler/runtime will **NOT** do all the optimisation for you.
- Profile your code yourself
 - Don't believe what anyone tells you. They're wrong.
- Profile on the hardware you want to run on
 - Don't profile on your laptop if you plan to run on ARCHER.
- Profile your code running the full-sized problem
 - The profile will almost certainly be qualitatively different for a test case.
- Keep profiling your code as you optimise
 - Concentrate your efforts on the thing that slows your code down.
 - This will change as you optimise.
 - So keep on profiling.





Theory

- Optimisation is an experimental process.
- You propose reasons why a code section is slow.
- Make corresponding changes.
- The results may surprise you
 - Need to revise the theory
- Never "optimise" without measuring the impact.





Exit?

- It is important to know when to stop.
- Each time you propose a code change consider:
 - The likely improvement
 - Code profile and Amdahl's law helps here.
 - Take account of how long much use you expect for the optimised code. Single use programs are rarely worth optimising.
 - The likely cost
 - Programming/debugging time.
 - Delay to starting simulation
 - "Damage" to the program





Changing code

- Many proposed changes will turn out not be useful.
- You may have to undo your changes.
 - At the very least keep old versions
 - Better to use revision control software.
- Always check the results are still correct !!
 - No point measuring performance if the results are wrong
 - A good test framework will help a lot





Damaging code

- Performance changes can damage other desirable aspects of the code.
 - Loss of encapsulation.
 - Loss of clarity
 - Loss of flexibility
- Think about down-side of changes.
- Look for alternative changes with same performance benefit but less damage.





Experimental frameworks

- Like any experiment, you need to keep good records.
- You will be generating large numbers of different versions of the code.
 - You need to know exactly what the different version were.
 - How you compiled them.
 - Did they get the correct answer.
 - · How did they perform.
- You may need to be able to re-run or reproduce your experiments
 - You discover a bug
 - A new compiler is released
 - A new hardware environment becomes available.
 - Etc.





Making things easier

- Keep everything under version control (including results)
- Script your tests so they are easy to run and give a clear yes/no answer.
- Write timing data into separate log-files in easily machine readable format.
- Keep notes.





Architecture trends

- Optimisation is the process of tuning a code to run faster in a particular Hardware and Software environment.
- The hardware environment consists of many different resources
 - FPU
 - Cache
 - Memory
 - I/O
- Any of these resources could be the limiting factor for code performance
 - Which one depends on the application





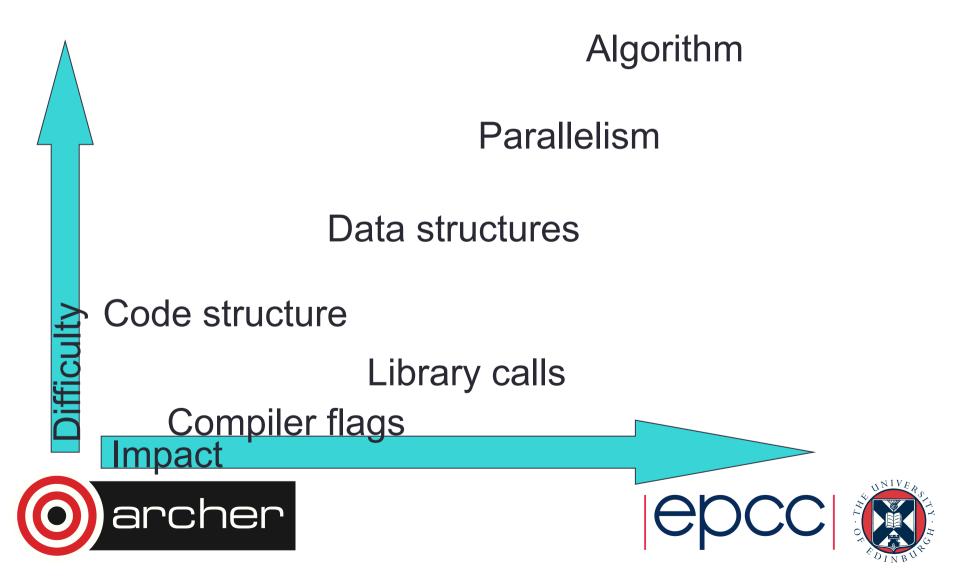
CPU resources

- In the early days of computing memory accesses were essentially free.
 - Optimisation consisted of reducing the instruction count.
- This is no longer the case, and is getting worse
 - CPU performance increases at approx. 80% per year (though recently this has been due to increasing core count rather than clock speed)
 - memory speed increases at approx. 7% per year
- Most HPC codes/systems are memory bandwidth limited.





Types of optimisation



Compiler flags

- Easiest thing to change are the compiler flags
- Most compilers will have good optimisation by default.
 - Some compiler optimisations are not always beneficial and need to be requested explicitly.
 - Some need additional guidance from user (e.g. inter-file in-lining)
 - Some break language standards and need to be requested explicitly
 - E.g. a/2 -> a*0.5 is contrary to Fortran standard but is usually safe.
 - Usually worthwhile to read compiler manual pages before optimising.





Library calls

- The easiest way to make a big impact on code performance is to re-use existing optimised code.
- Libraries represent large amount of development effort
 - Somebody else has put in the effort so you don't have to,
- Code libraries exist for commonly used functionality (e.g. linear algebra, FFTs etc.).
 - Often possible to access highly optimised versions of these libraries.
 - Even if the application code does not use a standard library it is often easy to re-write to use the standard calls.





Algorithm

- The biggest performance increases typically require a change to the underlying algorithm.
 - Consider changing an O(N) sort algorithm to a O(log(N)) algorithm.
 - This is a lot of work as the relevant code section usually needs a complete re-write.
- A warning
 - The complexity of an algorithm O(N), O(log(N)), O(N log(N)) etc. is related to number of operations and is not always a reliable indication of performance.
 - Pre-factor may make a "worse" algorithm perform better for the value of N of interest.
 - The "worse" algorithms may have much better cache re-use





Code structure

- Most optimisations involve changes to code structure
 - Loop unrolling
 - Loop fusion
 - routine in-lining.
- Often overlap with optimisations attempted by the compiler.
 - Often better to help the compiler to do this than perform change by hand.
- Easier to implement than data changes as more localised.
 - Performance impact is often also smaller unless the code fragment is a major time consumer.
- Performance improvement often at the expense of code maintainability.
 - Try to keep the unoptimised version up to date as well.





Helping the compiler

- Unless we write assembly code, we are always using a compiler.
- Modern compilers are (quite) good at optimisation
 - memory optimisations are an exception
- Usually much better to get the compiler to do the optimisation.
 - avoids machine-specific coding
 - compilers break codes much less often than humans
- Even modifying code can be thought of as "helping the compiler".





Compiler flags

- Typical compiler has hundreds of flags/options.
 - most are never used
 - many are not related to optimisation
- Most compilers have flags for different levels of general optimisation.
 - -01, -02, -03,....
- When first porting code, switch optimisation off.
 - only when you are satisfied that the code works, turn optimisation on, and test again.
 - but don't forget to use them!
 - also don't forget to turn off debugging, bounds checking and profiling flags...





Compiler flags (cont.)

- Note that highest levels of optimisation may
 - break your code.
 - give different answers, by bending standards.
 - make your code go slower.
- Always read documentation carefully.
- Isolate routines and flags which cause the problem.
 - binary chop
 - one routine per file may help





Code modification

- When flags and hints don't solve the problem, we will have to resort to code modification.
- Be aware that this may
 - introduce bugs.
 - make the code harder to read/maintain.
 - only be effective on certain architectures and compiler versions.
- Try to think about
 - what optimisation the compiler is failing to do
 - What additional information can be provided to compiler
 - how can rewriting help





Locals and globals

- Compiler analysis is more effective with local variables
- Has to make worst case assumptions about global variables
- Globals could be modified by any called procedure.
- Use local variables where possible
- Automatic variables are stack allocated: allocation is essentially free.
- In C, use file scope globals in preference to externals





Conditionals

- Even with sophisticated branch prediction hardware, branches are bad for performance.
- Try to avoid branches in innermost loops.
 - if you can't eliminate them, at least try to get them out of the critical loops.







Data types

- Performance can be affected by choice of data types
 - often a difference between 32-bit and 64-bit arithmetic (integer and floating point).
 - complicated by trade-offs with memory usage and cache hit rates
- Avoid unnecessary type conversions
 - e.g. int to long, float to double
 - N.B. some type conversions are implicit
 - However sometimes better than the alternative e.g.
 - Use DP reduction variable rather than increase array precision.





CSE

- Compilers are generally good at Common Subexpression Elimination.
- A couple of cases where they might have trouble:

Different order of operands

$$d = a + c$$

 $e = a + b + c$

Function calls

d	=	a	+	func(c)
е	=	b	+	func(c)





Register use

- Most compilers make a reasonable job of register allocation.
 - But only limited number available.
- Can have problems in some cases:
 - loops with large numbers of temporary variables
 - such loops may be produced by inlining or unrolling
 - array elements with complex index expressions
 - can help compiler by introducing explicit scalar temporaries, most compilers will use a register for an explicit scalar in preference to an implicit CSE.









Spilling

- If compiler runs out of registers it will generate spill code.
 - store a value and then reload it later on
- Examine your source code and count how many loads/ stores are required
- Compare with assembly code
- May need to distribute loops





Loop unrolling

- Loop unrolling and software pipelining are two of the most important optimisations for scientific codes on modern RISC processors.
- Compilers generally good at this.
- If compiler fails, usually better to try and remove the impediment, rather than unroll by hand.
 - cleaner, more portable, better performance
- Compiler has to determine independence of iterations





Loop unrolling

- Loops with small bodies generate small basic blocks of assembly code
 - Iot of dependencies between instructions
 - high branch frequency
 - little scope for good instruction scheduling
- Loop unrolling is a technique for increasing the size of the loop body
 - gives more scope for better schedules
 - reduces branch frequency
 - make more independent instructions available for multiple issue.





Loop unrolling

- Replace loop body by multiple copies of the body
- Modify loop control
 - take care of arbitrary loop bounds
- Number of copies is called unroll factor

```
Example:

do i=1,n-3,4

a(i)=b(i)+d*c(i)

a(i+1)=b(i+1)+d*c(i+1)

a(i+2)=b(i+2)+d*c(i+2)

a(i+3)=b(i+3)+d*c(i+3)

end do

do j = i,n

a(j)=b(j)+d*c(j)

end do

Concher
```

- Remember that this is in fact done by the compiler at the IR or assembly code level.
- If the loop iterations are independent, then we end up with a larger basic block with relatively few dependencies, and more scope for scheduling.
 - also reduce no. of compare and branch instructions
- Choice of unroll factor is important (usually 2,4,8)
 - if factor is too large, can run out of registers
- Cannot unroll loops with complex flow control
 - hard to generate code to jump out of the unrolled version at the right place





Impediments to unrolling

- Function calls
 - except in presence of good interprocedural analysis and inlining

Conditionals

- especially control transfer out of the loop
- Lose most of the benefit anyway as they break up the basic block.
- Pointer/array aliasing
 - Compiler can't be sure different values don't overlap in memory





Example

```
for (i=0;i<ip;i++) {
    a[indx[i]] += c[i] * a[ip];
}</pre>
```

- Compiler doesn't know that a[indx[i]] and a[ip] don't overlap
- Could try hints
 - tell compiler that indx is a permutation
 - tell compiler that it is OK to unroll
- Or could rewrite:

```
tmp = a[ip];
for (i=0;i<ip;i++) {
    a[indx[i]] += c[i] * tmp;
}
```







Inlining

Compilers very variable in their abilities

- Hand inlining possible
 - very ugly (slightly less so if done via pre-processor macros)
 - causes code replication
- Compiler has to know where the source of candidate routines is.
 - sometimes done by compiler flags
 - · easier for routines in the same file
 - try compiling multiple files at the same time
- Very important for OO code
 - OO design encourages methods with very small bodies
 - inline keyword in C++ can be used as a hint





Vector Instructions (Vectorisation)

- Modern CPUs can perform multiple operations each cycle
 - Use special SIMD (Single Instruction Multiple Data) instructions
 - e.g. SSE, AVX
 - Operate on a "vector" of data
 - typically 2 or 4 double precision
 - potentially gives speedup in floating point operations
 - Usually only one loop is vectorisable in loop nest
 - And most compilers only consider inner loop





- Optimising compilers will use vector instructions
 - Relies on code being vectorisable
 - ...or in a form that the compiler can convert to be vectorisable
 - Some compilers are better at this than others
 - But there are some general guidelines about what is likely to work...





Requirements for vectorisation

- Loops must have determinable (at run time) trip count
 - rules out most while loops
- Loops must not contain function/subroutine calls
 - unless the call can be inlined by the compiler
 - maths library functions usually OK
- Loops must not contain braches or jumps
 - guarded assignments may be OK

• e.g. if (a[i] != 0.0) b[i] = c * a[i];

 Loop trip counts needs to be long, or else a multiple of the vector length





- Loops must no have dependencies between iterations
 - reductions usually OK, e.g. sum += a[i];
 - avoid induction variables e.g. indx += 3;
 - USE restrict
 - may need to tell the compiler if it can't work it out for itself
- Aligned data is best
 - e.g. AVX vector loads/stores operate most effectively on 32-bytes aligned address
 - need to either let the compiler align the data....
 - .. or tell it what the alignment is
- Unit stride through memory is best





Multiple Optimisation steps

- Sometimes multiple optimisation steps are required.
 - Multiple levels of in-lining.
 - In-lining followed by loop un-rolling followed by CSE.
- The compiler may not be able to perform all steps at the same time
 - You may be able to help the compiler by performing some of the steps by hand.
 - Look for the least damaging code change that allows the compiler to complete the rest of the necessary changes.
 - Ideally try each step in isolation before attempting to combine hand-optimisations.





Data structures

- Changing the programs data structures can often give good performance improvements
 - These are often global changes to the program and therefore expensive.
 - Code re-writing tools can help with this.
 - Easier if data structures are reasonably opaque, declared once
 - objects, structs, F90 types, included common blocks.
 - As memory access is often the major performance bottleneck the benefits can be great.
 - Improve cache/register utilisation.
 - Avoid pointer chasing
 - May be able to avoid memory access problems by changing code structure in key areas instead.





Programmer's perspective:

- Memory structures are the programmers responsibility
 - At best the compiler can add small amounts of padding in limited circumstances.
 - Compilers can (and hopefully will) try to make best use of the memory structures that you specify (e.g. uni-modular transformations)
- Changing the memory structures you specify may allow the compiler to generate better code.





Arrays

- Arrays are large blocks of memory indexed by integer index
- Probably the most common data structure used in HPC codes
- Good for representing regularly discretised versions of dense continuous data

 $f(x,y,z) \rightarrow F[i][j][k]$





Arrays

- Many codes loop over array elements
 - Data access pattern is regular and easy to predict
- Unless loop nest order and array index order match the access pattern may not be optimal for cache re-use.
 - Compiler can often address these problems by transforming the loops.
 - But sometimes can do a better job when provided with a more cache-friendly index order.





What can go wrong

- Poor cache/page use
 - Lack of spatial locality
 - Lack of temporal locality
 - cache thrashing
- Unnecessary memory accesses
 - pointer chasing
 - array temporaries
- Aliasing problems
 - Use of pointers can inhibit code optimisation





Reducing memory accesses

- Memory accesses are often the most important limiting factor for code performance.
 - Many older codes were written when memory access was relatively cheap.
- Things to look for:
 - Unnecessary pointer chasing
 - pointer arrays that could be simple arrays
 - linked lists that could be arrays.
 - Unnecessary temporary arrays.
 - Tables of values that would be cheap to re-calculate.





Utilizing caches

- Want to use all of the data in a cache line
 - loading unwanted values is a waste of memory bandwidth.
 - structures are good for this
 - or loop fastest over the corresponding index of an array.
- Place variables that are used together close together
 - Also have to worry about alignment with cache block boundaries.
- Avoid "gaps" in structures
 - In C structures may contain gaps to ensure the address of each variable is aligned with its size.





Arrays and caches

Bad: non-contiguous memory accesses

```
do i=1,n
    do j=1,m
        a(i,j) = b * c(i,j)
        end do
end do
```

Good: contiguous memory accesses

```
do j=1,m
    do i=1,n
        a(i,j) = b * c(i,j)
        end do
end do
```

```
for (j=0;i<m;j++) {
    for (i=0;i<n;i++) {
        a[i][j] = b * c[i][j];
    }
}</pre>
```

```
for (i=0;i<n;i++) {
    for (j=0;j<m;j++) {
        a[i][j] = b * c[i][j];
    }
}</pre>
```



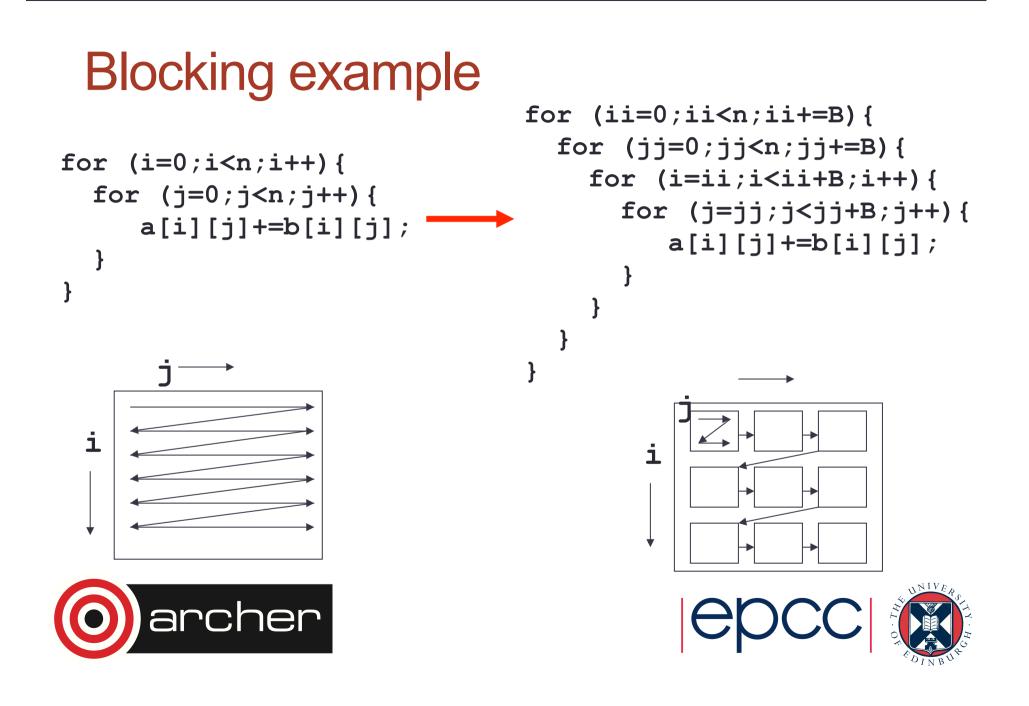


Cache blocking

- A combination of:
 - strip mining (also called loop blocking, loop tiling...)
 - loop interchange
- Designed to increase data reuse:
 - temporal reuse: reuse array elements already referenced
 - spatial reuse: good use of cache lines
- Many ways to block any given loop nest
 - Which loops should be blocked?
 - What block size(s) will work best?







Further cache optimisations

- If multiple loop nests process a large array
 - First element of array will be out of cache when start second loop nest
- Improving cache use
 - Consider fusing the loop nests
 - Completely: just have one loop nest
 - Partial: have one outer loop, containing multiple inner loops
 - Beware that too much fusion can result in lots of temporaries and cause the compiler to run out of registers....





Original code	Complete fusion	Partial fusing
<pre>do j = 1, Nj do i = 1, Ni a(i,j)=b(i,j)*2 enddo enddo</pre>	<pre>do j = 1, Nj do i = 1, Ni a(i,j)=b(i,j)*2 a(i,j)=a(i,j)+1 enddo enddo</pre>	<pre>do j = 1, Nj do i = 1, Ni a(i,j)=b(i,j)*2 enddo do i = 1, Ni a(i,j)=a(i,j)+1</pre>
<pre>do j = 1, Nj do i = 1, Ni a(i,j)=a(i,j)+1 enddo enddo</pre>		enddo enddo





Further cache optimisations

- Perhaps cache block before fusing
 - Fuse one or more of the outer blocking loops
- If multiple subprograms process the array
 - Remove one or more outer loops (or all loops) from subprograms
 - Haul loop into parent routine, pass in index values instead
 - Might want to ensure that compiler is inlining this routine
 - This technique is very useful if you want to use OpenMP/OpenACC
- Beware of Fortran
 - array syntax often bad
 - a(:,:)=b(:,:)*2
 - a(:,:)=a(:,:)+1
 - compiler unlikely to fuse any loops





Original code

CALL sub1(a,b) CALL sub2(a)

```
SUBROUTINE sub1(a)
do j=1,Nj
do i=1,Ni
a(i,j)=b(i,j)*2
enddo
enddo
END SUBROUTINE sub1
```

After hauling

do j = 1, Nj
 CALL sub1(a,b,j)
 CALL sub2(a,j)
enddo

SUBROUTINE sub1(a,j)
do i=1,Ni
 a(i,j)=b(i,j)*2
enddo
END SUBROUTINE sub1





Optimising for TLB

- Aim to reuse data on a page
 - i.e. treat similarly to a cache

Standard-sized pages are 4kB

- But you can use larger "huge" pages
 - 128kB, 512kB, 2MB,... 64MB
- Almost always benefit HPC applications
 - regular data accesses
 - huge pages give fewer TLB misses
- Huge pages can also help communication performance





Prefetch

- Some processors (including Ivy Bridge) prefetch automatically
- Regular access patterns are recognized and cache lines fetched in advance.
 - Usually only works for contiguous sequence of cache misses.
- Processor has a set of stream buffers
 - Each holds address of an active stream
 - Loads to the current block causes the next block to be prefetched and the stream address to be updated.
 - Streams are established by series of cache misses to consecutive locations





Using streams

- To utilize stream hardware use linear access patterns where possible
 - Only the order of cache block accesses needs to be linear, not each word access.
- Most loops will require multiple streams
 - If the loop requires more streams than are supported in hardware no prefetching will take place for some of the loads.
 - Consider splitting the loop.
- Prefetching typically cannot cross OS page boundaries
 - huge pages may help





Pointer aliasing

- Pointers are variables containing memory addresses.
 - Pointers are useful but can seriously inhibit code performance.
- Compilers try very hard to reduce memory accesses.
 - Only loading data from memory once.
 - Keep variables in registers and only update memory copy when necessary.
- Pointers could point anywhere, so to be safe compiler will:
 - Reload all values after write through pointer
 - Synchronize all variables with memory before read through pointer





Pointers and Fortran

- F77 had no pointers
- Arguments passed by reference (address)
 - Subroutine arguments are effectively pointers
 - But it is illegal Fortran if two arguments overlap
- F90/F95 has restricted pointers
 - Pointers can only point at variables declared as a "target" or at the target of another pointer
 - Compiler therefore knows more about possible aliasing problems
- Try to avoid F90 pointers for performance critical data structures.





Pointers and C

- In C pointers are unrestricted
 - Can therefore seriously inhibit performance
- Almost impossible to do without pointers
 - malloc requires the use of pointers.
 - Pointers used for call by reference. Alternative is call by value where all data is copied!
- Use the C99 restrict keyword where possible
- ... or else use compiler flags
- Explicit use of scalar temporaries may also reduce the problem





Key points to remember

- Optimisation tunes a code for a particular environment
 - Not all optimisations are portable.
- Optimisation is an experimental process.
- Need to think about cost/benefit of any change.
- Always verify the results are correct.



