



EPSRC

ARCHER Single Node Optimisation

Vectorisation

Slides contributed by Cray and EPCC



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 floats (on Ivy Bridge)
 - 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 branches 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 not 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



Did my loop get vectorised?

- Always check the compiler output to see what it did
 - CCE: `-hlist=a`
 - GNU: `-fdump-tree-vect-all=<filename>`
 - Intel: `-opt-report3`
 - or (for the hard core) check the assembler generated
- Clues from CrayPAT's HWPC measurements
 - `export PAT_RT_HWPC=13 or 14 # Floating point operations SP,DP`
 - Complicated, but look for ratio of operations/instructions > 1
 - expect 4 for pure AVX with double precision floats



Example

```
16.  + 1-----<   do j = 1,N
17.    1             x = xinit
18.  + 1 r4-----<   do i = 1,N
19.    1 r4          x = x + vexpr(i,j)
20.    1 r4          y(i) = y(i) + x
21.    1 r4----->   end do
22.    1----->     end do
```

1.497ms

ftn-6254 ftn: VECTOR File = bufpack.F90, Line = 16

A loop starting at line 16 was **not vectorized** because a recurrence was found on "y" at line 20.

ftn-6005 ftn: SCALAR File = bufpack.F90, Line = 18

A loop starting at line 18 was **unrolled 4 times**.

ftn-6254 ftn: VECTOR File = bufpack.F90, Line = 18

A loop starting at line 18 was not vectorized because a recurrence was found on "x" at line 19.



```

38.   Vf-----<   do j = 1,N
39.   Vf             x(j) = xinit
40.   Vf----->   end do
41.
42.   ir4-----<   do j = 1,N
43.   ir4 if--<     do i = 1,N
44.   ir4 if         x(j) = x(j) + vexpr(i,j)
45.   ir4 if         y(i) = y(i) + x(j)
46.   ir4 if-->     end do
47.   ir4----->   end do

```

x promoted to vector:
trade slightly more memory
for better performance

1.089ms
-37%

ftn-6007 ftn: SCALAR File = bufpack.F90, Line = 42

A loop starting at line 42 was **interchanged** with the loop starting at line 43.

ftn-6004 ftn: SCALAR File = bufpack.F90, Line = 43

A loop starting at line 43 was **fused** with the loop starting at line 38.

ftn-6204 ftn: VECTOR File = bufpack.F90, Line = 38

A loop starting at line 38 was **vectorized**.

ftn-6208 ftn: VECTOR File = bufpack.F90, Line = 42

A loop starting at line 42 was **vectorized** as part of the loop starting at line 38.

ftn-6005 ftn: SCALAR File = bufpack.F90, Line = 42

A loop starting at line 42 was **unrolled 4 times**.

OpenMP 4.0 SIMD directives

- Many compilers support their own sets of directives to assist the compiler to vectorise loops.
 - useful but not portable
- OpenMP 4.0 contains a standardised set of directives
- Currently supported by Intel and GNU compilers on ARCHER
 - Cray coming soon.....



Portable SIMD directives

- Use **simd** directive to indicate a loop should be vectorised

```
#pragma omp simd [clauses]
```

or

```
!$omp simd [clauses]
```

- Executes iterations of following loop in SIMD chunks
- Loop is *not* divided across threads
- SIMD chunk is set of iterations executed concurrently by SIMD lanes
- Not a hint! Programmer is asserting independence of iterations.



- Clauses control data environment, how loop is partitioned
- **safelen(length)** limits the number of iterations in a SIMD chunk.
- **linear** lists variables with a linear relationship to the iteration space (induction variables)
- **aligned** specifies byte alignments of a list of variables
- **private**, **lastprivate**, **reduction** and **collapse** have usual meanings.
- Also **declare simd** directive to generate SIMDised versions of functions.
- Can be combined with loop constructs (parallelise and vectorise)
 - **#pragma omp for simd**

