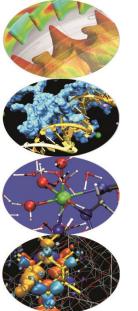


Compilers and Optimisation

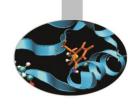


Andrew Emerson





Introduction

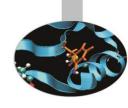


- The hardware components of modern supercomputers are capable of providing substantial computing power
- To obtain high performing applications we require:
 - Efficient programming
 - A good understanding of the compilers and how that optimize code for the underlying hardware
 - Tools such as profilers, debuggers, etc, in order to obtain the best performance





The compiler

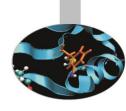


- There are many compilers available and for all computer operating systems (e.g. Linux, Windows or Macintosh).
- As well as free compilers from the GNU project there are also various commercial compilers (e.g. Portland or Intel)
- Some compilers are provided with the hardware (e.g. IBM xlf)





Compilers and interpreters

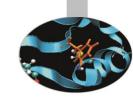


- Interpreted languages
 - The code is "translated" statement-by-statement during the execution
 - Easier on the programmer, modifications can be made quickly but optimisations between different statements (almost) impossible
 - Used for scripting languages (bash, Perl, PHP, ..)
- Compiled languages
 - Entire program is translated before execution
 - Optimisations between different parts of the program possible.
 - HPC languages such as FORTRAN, C and C++





What does the compiler do?

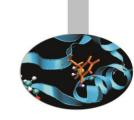


- Translates source code into machine code, if no syntax errors found. Warnings for potential semantic problems.
- Can attempt to optimise the code. Optimisations can be:
 - Language dependent or independent
 - Hardware dependent (e.g. CPU, memory, cache)
- Compilers are very sophisticated software tools but cannot replace human understanding of what the code should do.





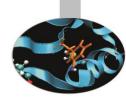
Pre-processing, compiling and linking



- "Compiling" a program is actually a three stage process:
 - Pre-processing to replace MACROs (#define), code insertions (#include), code selections (#ifdef, #if).
 Originally C/C++ but also used in FORTRAN.
 - Compilation of the source code into object files organised collections of symbols referring to variables and functions.
 - 3. Linking of the object files, together with any external libraries to create the executable (if all referred objects are resolved).
- For large projects usual to separate the compiling and linking phases.
- Code optimisations are mainly done during compilation, but how a program is linked may also affect performance (e.g. BG/Q).



Which compiler?

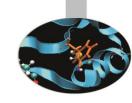


- Common compiler suites include:
 - GNU (gcc, gfortran,...)
 - Intel (icc, icpc, icc)
 - IBM (xlf, xlc, xlC)
 - Portland (pgf90, pgcc, pgCC)
 - LLVM (Clang)
- If I have a choice, which one?
 - Various things to consider. For performance vendorspecific (e.g. Intel on Intel CPUs or KNL) but many tools have been developed with GNU.





What does the compiler do?

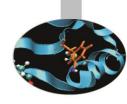


- The compiler can perform many optimisations including:
 - Register allocation
 - Dead and redundant code removal
 - Common subexpression elimination (CSE)
 - Strength reduction (e.g. replacing an exponentiation within a loop with a multiplication)
 - Inlining
 - Loop optimisations such as index reordering, loop pipelining, unrolling, merging
 - Cache blocking





What the compiler does

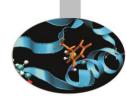


- What the compiler cannot do:
 - Understand dependencies between data with indirect addressing
 - Non-integer or complex strength reduction
 - Optimize by Unrolling/Merging/Blocking with
 - Calls to functions or subroutines
 - I/O statements or calls within the code
 - Optimize variables with values known only at run-time
- Compilers are generally conservative, i.e. will not optimise if strong risk of obtaining incorrect results *unless* forced to by the user either with compiler directives or options.
- Still sometimes happens that codes give wrong results, even with minor optimisations.





C/FORTRAN Compilers available at Cineca (Marconi)



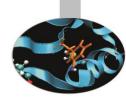
```
$ module avail
gnu/6.1.0
intel/pe-xe-2016--binary
intel/pe-xe-2017--binary(default)
intelmpi/2017--binary(default)
intelmpi/5.1--binary
jre/1.8.0_111--binary
openmpi/1-10.3--gnu--6.1.0(default)
openmpi/1-10.7--gnu--6.1.0
openmpi/1.10.3-threadmultiple--gnu--6.1.0
```

- Gnu, Intel and PGI compilers are available for C/C++ and Fortran.
- Two implementations of MPI: IntelMPI and OpenMPI.
- For applications currently recommend Intel compilers with IntelMPI, but for non-CPU intensive programs probably GNU compilers will be easier (more common).





Optimisation options - Intel



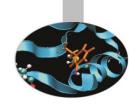
icc (or ifort) -03

- Automatic vectorization (use of packed SIMD instructions)
- Loop interchange (for more efficient memory access)
- Loop unrolling (more instruction level parallelism)
- Prefetching (for patterns not recognized by h/w prefetcher)
- Cache blocking (for more reuse of data in cache)
- Loop peeling (allow for misalignment)
- Loop versioning (for loop count; data alignment; runtime dependency tests)
- Memcpy recognition (call Intel's fast memcpy, memset)
- Loop splitting (facilitate vectorization)
- Loop fusion (more efficient vectorization)
- Scalar replacement (reduce array accesses by scalar temps)
- Loop rerolling (enable vectorization)
- Loop reversal (handle dependencies)
 28/11/2017 Compilers and optimisation





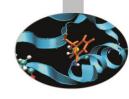
Optimisation options



- Compilers give the possibility of specifying optimisation options at compile time, together with the other options.
- These are either general optimisation levels or specific flags related to the underlying hardware.
- Some options can greatly increase the compilation time so one reason for starting with a low optimisation level during code development.





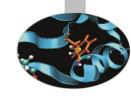


- -O0: no optimisation, the code is translated literally
- -O1, -O2: local optimisations, compromise between compilation speed, optimisation, code accuracy and executable size (usually default)
- -O3: high optimisation, can alter the semantics of the program (hence not used for debugging)
- -O4 or higher: Aggressive optimisations, depending on hardware.





CACan I just leave it to the compiler to optimise my code?



- Example: matrix-matrix multiplication (1024x1024), double precision, FORTRAN.
- Two systems:
 - FERMI: (IBM BG/Q Power A2, 1.6Ghz)
 - PLX: (Xeon Westmere CPUs, 2.4 Ghz)

FERMI xlf PLX -ifort

Option	Seconds	MFlops	
-00	65.78	32.6	
-02	7.13	301	
-03	0.78	2735	
-04	55.52	38.7	
-05	0.65	3311	

Option	Seconds	MFlops	
-00	8.94	240	
-02	1.41	1514	
-03	0.72	2955	
-04	0.33	6392	
-05	0.32	6623	



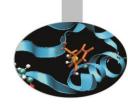
Can I just leave it to the compiler to optimise my code?

- To find out what is going on can invoke the -qreport option of xlf. It tells us what the compiler is actually doing.
- On Fermi, for –O4 the option tells us that the optimiser follows a different strategy:
 - The compiler recognises the matrix-matrix product and substitutes the code with a call to a library routine __xl_dgemm
 - This is quite slow, particularly compared to the IBM optimised library (ESSL).
 - Intel uses a similar strategy, but uses instead the efficient MKL library
- Moral? Increasing the optimisation level doesn't always increase performance. Must check each time.





Optimising Loops



- Many HPC programs consume resources in loops where there are array accesses.
- Since main memory accesses are expensive principle goal when optimising loops is maximise data locality so that the cache can be used. Another goal is to aid vectorisation.
- For simple loops the compiler can do this but sometimes it needs help.
- Important to remember differences between FORTRAN and C for array storage.
- But should always test the performance. For small arrays, in particular, the various optimisations may give worse results.





Loop optimisations

- First rule: always use the correct types for loop indices. Otherwise the compiler will have to perform real to integer conversions.
- FORTRAN compilers may indicate an error or warning, but usually tolerated

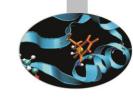
```
real :: i,j,k
....

do j=1,n
    do k=1,n
    do i=1,n
        c(i,j)=c(i,j)+a(i,k)*b(k,j)
    enddo
    enddo
enddo
```

Compilation	integer	real
PLX gfortran –O0	9.96	8.37
PLX gfortran –O3		
	0.75	2.63
PLX ifort -O0	6.72	8.28
PLX ifort -O3	0.33	1.74
Plx pgif90	4.73	4.85
Plx pgif90 -fast	0.68	2.3
Fermi bglxlf –O3	64.78	104.1
Fermi bgxlf –O3	0.64	12.38



Loop optimisations: index reordering



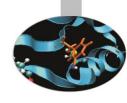
For simple loops, the compiler optimises well

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

Compilation	J-k-i	i-k-j
Ifort –O0	6.72	21.8
Ifort –fast	0.34	0.33



Loop optimisations – index reordering



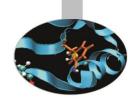
- For more complex, nested loops optimised performances may differ.
- Important to understand the cache mechanism!

```
do jj = 1, n, step
  do kk = 1, n, step
    do ii = 1, n, step
      do j = jj, jj+step-1
       do k = kk, kk+step-1
         do i = ii, ii+step-1
           c(i,j) = c(i,j) + a(i,k)*b(k,j)
         enddo
       enddo
      enddo
    enddo
  enddo
enddo
```

Compilation	j-k-i	i-k-j	
(PLX) ifort -O0	10	11.5	
(PLX) ifort -fast	1.	2.4	



Loop optimisations -cache blocking



If the a,b,c, arrays fit into the cache, performance is fast

```
for (i = 0; i < N; i = i+1)
  for (j = 0; j < N; j = j+1) {
    r = 0;
    for (k = 0; k < N; k = k+1){
        r = r + y[i][k]*z[k][j];
    }
    x[i][j] = r;
};</pre>
```

If not then performance is slow. By adding loops, can reduce data held such that it fits into cache.

```
for (jj = 0; jj < N; jj = jj+B)
  for (kk = 0; kk < N; kk = kk+B)
    for (i = 0; i < N; i = i+1)
      for (j = jj; j < min(jj+B-1,N); j = j+1) {
        r = 0;
      for (k = kk; k < min(kk+B-1,N); k = k+1) {
        r = r + y[i][k]*z[k][j];
      }
      x[i][j] = x[i][j] + r;
    };</pre>
```

B=blocking factor





Loop optimisations – unrolling (or unwinding

- Aim to reduce loop overhead (e.g. loop control instructions) by reducing iterations. Can also reduce memory accesses, and aid vectorisation.
- Can be done by replicating the code inside the loop.
- Most effective when the computations in the loop can be simulated by the compiler (e.g. stepping sequentially through an array).
 Clearly, the no. of iterations should be known before execution.

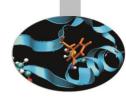
```
for(int
i=0;i<1000;i++)
a[i] = b[i] + c[i];
```

in some cases can eliminate a loop altogether

```
for(int i=0;i<1000;i+=4) {
    a[i] = b[i] + c[i];
    a[i+1] = b[i+1] + c[i+1];
    a[i+2] = b[i+2] + c[i+2];
    a[i+3] = b[i+3] + c[i+3];
}</pre>
```







- A loop transformation which replaces multiple loops with a single one (to avoid loop overheads and aid cache use).
- Possible when two loops iterate over the same range and do not reference each other's data. (unless "loop peeling" is used)
- Doesn't always improve performance sometimes cache is better used in two loops (Loop fission)

```
/* Unoptimized */
for (i = 0; i < N; i = i + 1)
  for (j = 0; j < N; j = j + 1)
    a[i][j] = 2 * b[i][j];

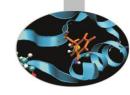
for (i = 0; i < N; i = i + 1)
  for (j = 0; j < N; j = j + 1)
    c[i][j] = K*b[i][j]+ d[i][j]/2</pre>
```

```
/* Optimized */
for (i = 0; i < N; i = i + 1)
  for (j = 0; j < N; j = j + 1)
  a[i][j] = 2 * b[i][j];
  c[i][j] = K*b[i][j]+d[i][j]/2</pre>
```





Loop optimisations - fission



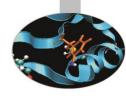
- The opposite of Loop fusion, i.e. splitting a single loop into multiple loops.
- Often used when:
 - 1. computations in single loop become too many(which can lead to "register spills").
 - 2. If the loop contains a conditional: create 2 loops, one without conditional for vectorisation.
 - 3. Improve memory locality.

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





Array of Structures (AoS) vs Structure of Arrays (SoA)



- Depends on access patterns, but for vectorised C/C++ usually preferable to have SoA rather than AoS since array elements are contiguous in memory.
- SoA also usually uses less memory because of data alignment.

```
// AoS
struct node {
    float x,y,z;
// other data
};
struct node NODES[N];
```

```
// SoA
struct node {
   float x[N];
   float y[N];
   float z[N];
//other data
};
struct node NODES;
```



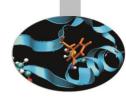


Example

```
// Array of structures
                                     // Struct of Arrays
  struct node {
                                     struct node {
      float x,y,z;
                                         float x[N];
      int n;
                            icc -02 -opt-report 2 -o soa soa.c -lm
  };
                            soa.c(22:1-22:1):VEC:main: LOOP WAS VECTORIZED
                            soa.c(29:1-29:1):VEC:main: LOOP WAS VECTORIZED
  struct node NODES[N];
                                     struct node NODES;
  for (i=0;i<N;i++) {
     NODES[i].x=1;
                                     for (i=0;i<N;i++) {
     NODES[i].y=1;
                                        NODES.x[i]=1;
     NODES[i].z=1;
                                        NODES.y[i]=1;
  for (i=0; i<N; i++) {
                                        NODES.z[i]=1;
     x=NODES[i].x;
     y=NODES[i].y;
                                     for (i=0; i<N; i++) {
      z=NODES[i].z;
                                        x=NODES.x[i];
      sum+=sqrtf(x*x+y*y+z*z);
                                        y=NODES.y[i];
icc -02 -opt-report 2 -o aos aos.c -lm
aos.c(18:1-18:1):VEC:main: loop was not vectorized: not inner loop
aos.c(19:4-19:4):VEC:main: loop was not vectorized: low trip count
aos.c(25:1-25:1):VEC:main: LOOP WAS VECTORIZED
```



Vectorisation



 Modern processors have dedicated circuits and SIMD instructions for operating on blocks of data ("vectors") rather than single data items.

$$c(0) = a(0) + b(0)$$

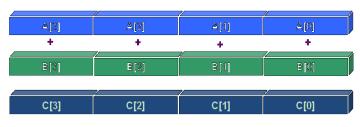
 $c(1) = a(1) + b(1)$
 $c(2) = a(2) + b(2)$
 $c(3) = a(3) + b(3)$

non vectorised

e.g. 3 x 32-bit unused integers



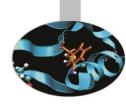
vectorised







Vectorisation evolution

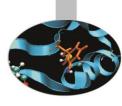


- SSE: 128 bit registers (intel Core AMD Opteron)
 - 4 floating/integer operations in single precision
 - 2 floating/integer operations in double precision
- AVX: 256 bit registers (intel Sandy Bridge AMD Bulldozer)
 - 8 floating/integer operations in single precision
 - 4 floating/integer operations in double precision
- MIC: 512 bit registers (Intel Knights Corner 2013)
 - 16 floating/integer operations in single precision
 - 8 floating/integer operations in double precision
- AVX: 512 bit registers KNL (Knight's Landing)
 - 16 FP (single), 8FP (double) but with AVX vector instructions





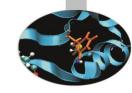
Vectorisation



- Loop vectorisation can increase dramatically the performance.
- But to be vectorisable a loop must obey certain criteria, in particular the absence of dependencies between separate iterations.
- Other criteria include:
 - Countable (constant number of iterations)
 - Single entry/exit points (no branches, unless implemented as masks)
 - Only the internal loop of a nested loop
 - No function calls (unless inlined or using a vector version of the function)
- Note that AVX can different numerical results (e.g. Fused Multiply Addition)



Vectorisation Algorithms



- Different algorithms performing the same task can behave differently wrt vectorisation.
 - Gauss-Seidel: dipendency between iterations, not vectorisable.

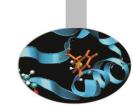
```
for( i = 1; i < n-1; ++i )
  for( j = 1; j < m-1; ++j )
    a[i][j] = w0 * a[i][j] +
    w1*(a[i-1][j] + a[i+1][j] + a[i][j-1] + a[i][j+1]);</pre>
```

Jacobi: no dependency, vectorisable.

```
for( i = 1; i < n-1; ++i )
  for( j = 1; j < m-1; ++j )
    b[i][j] = w0*a[i][j] +
    w1*(a[i-1][j] + a[i][j-1] + a[i+1][j] + a[i][j+1]);
for( i = 1; i < n-1; ++i )
  for( j = 1; j < m-1; ++j )
    a[i][j] = b[i][j];</pre>
```



Helping the vectoriser



- Some "coding tricks" can block vectorisation:
 - vectorisable

```
for( i = 0; i < n-1; ++i ) {
    b[i] = a[i] + a[i+1];
}</pre>
```

non vectorisable because x is needed for the next iteration.

```
x = a[0];
for(i = 0; i < n-1; ++i){
    y = a[i+1];
    b[i] = x + y;
    x = y;
}</pre>
```

- If the code hasn't vectorised then you can help the compiler by:
 - modifying the code to make it vectorisable
 - inserting compiler directives to force the vectorisation





Helping the vectoriser

- If the programmer knows that a dependency indicated by the programme is only apparent then the vectorisation can be forced with compilerdependent directives.
 - Intel FOTRAN: !DIR\$ simd
 - Intel C:#pragma simd
- so if we know that inow ≠ inew then there is in fact no dependency

```
do k = 1,n
!DIR$ simd
  do i = 1, 1
   x02 = a02(i-1,k+1,inow)
   x04 = a04(i-1,k-1,inow)
   x05 = a05(i-1,k,inow)
   x06 = a06(i, k-1, inow)
   x19 = a19(i, k, inow)
   rho = +x02+x04+x05+x06+x11+x13+x14+x15+x19
   a05(i,k,inew) = x05 - omega*(x05-e05) + force
```



Vectorisation can be difficult...

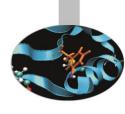
One of the following code snippets vectorises, the other one doesn't

```
subroutine vec
integer, parameter ::n=1000
integer :: i
real :: a(n),b(n),c(n)
do i=2,n
   a(i-1)=a(i)+1
enddo
end subroutine
```

```
subroutine vec
integer, parameter ::n=1000
integer :: i
real :: a(n),b(n),c(n)
do i=2,n
   a(i) = a(i-1) + 1
end do
end subroutine
```



Inlining



- A manual or compiler optimisation which replaces a call to the function with the body of the function itself.
 - eliminates the cost of the function call and can improve instruction cache performance
 - makes inter-procedure optimisation easier
- In C/C++ the keyword inline is a "suggestion"
- Not every function is "inlineable" depends on the compiler.
- Can cause increase in code size, particularly for large functions.
- Intel: -inline=n (0=disable, 1=keyword, 2=compiler decides)
- GNU: -finline-functions, -finline-limit=n
- In some compilers activated at high optimisation levels





Common Subexpression Elimination (CSE)

- Sometimes identical expressions are calculated more than once.
 When this happens may be useful to replace them with a variable holding the value.
- This

$$A = B+C+D$$

$$E = B+F+C$$

requires 4 sums. But the following

$$A = (B+C) + D$$

$$E = (B+C)+D$$

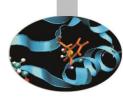
requires 3 sums.

- Careful: the floating point result may not be identical
- Another use is to replace an array element with a scalar to avoid multiple array lookups.





CSE and function calls



- By altering the order of the calls the compiler doesn't know if the result is affected (possible side-effects)
- 5 function calls, 5 products

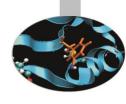
```
x=r*sin(a)*cos(b);
y=r*sin(a)*sin(b);
z=r*cos(a);
```

4 function calls, 4 products (1 temporary variable)

```
temp=r*sin(a)
x=temp*cos(b);
y=temp*sin(b);
z=r*cos(a);
```



CSE: Limitations

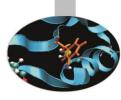


- Loops which are too big:
 - The compiler works with limited window sizes: it may not detect which quantity to re-use
- Functions:
 - If I change the order of the functions do I still get the same result?
- Order and evaluations:
 - Only at high levels of optimisation does the compiler change the order of operations (usually –O3 and above).
 - In some expressions it is possible to inhibit the mechanism with parantheses (the programmer is always right!).
- Since intermediate values are used will increase use of registers (risk of "register spilling").





Optimisation Reports



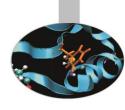
Compiler dependent. Intel provides various useful options:

```
-opt-report[n] n=0(none),1(min),2(med),3(max)
-opt-report-file<file>
-vec-report[n] n=0(none),1(min),2,3,4,5,6,7(max)
....
```

- The GNU suite does not provide exactly equivalent options.
 - The best option is to specify: -fdump-tree-all
 - which prints out alot of stuff (but not exactly in user-friendly form).



Static and dynamic allocation



- Static allocation in principle can help the compiler optimise by providing more information. But
 - the code becomes more rigid
 - in parallel computing dynamic allocation is very useful

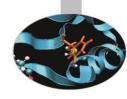
```
integer :: n
parameter(n=1024)
real a(1:n,1:n)
real b(1:n,1:n)
real c(1:n,1:n)
```

```
real, allocatable, dimension(:,:) :: a
real, allocatable, dimension(:,:) :: b
real, allocatable, dimension(:,:) :: c
print*,'Enter matrix size'
read(*,*) n
allocate(a(n,n),b(n,n),c(n,n))
```









- For recent compilers, performances are often similar for static and dynamic allocations.
 - e.g. matrix-matrix multiplication

Compiler	Static	Dynamic
PLX ifort -O0	6.72	18.26
PLX ifort –fast	0.34	0.35

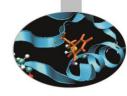
- Note that static allocations use the "stack", which is generally limited.
- In the bash shell you can use the ulimit command to see and (possibly) set the stack.

```
ulimit -a ulimited
```





Dynamic allocation in C



- C doesn't have a native 2-d array (unlike FORTRAN) but instead uses arrays of arrays.
- Static allocation guarantees all the values are contiguous in memory

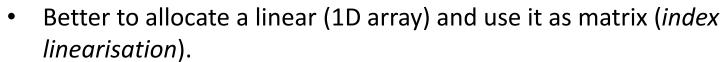
```
double A[nrows][ncols];
```

Dynamic allocation can be inefficient, if not done carefully

```
/* Inefficient array allocation */
/* Allocate a double matrix with many malloc */
double** allocate_matrix(int nrows, int ncols) {
   double **A;
   /* Allocate space for row pointers */
   A = (double**) malloc(nrows*sizeof(double*));
   /* Allocate space for each row */
   for (int ii=1; ii<nrows; ++ii) {
        A[ii] = (double*) malloc(ncols*sizeof(double));
   }
return A;
}</pre>
```



Dynamic array allocation in C/2



```
/* Allocate a double matrix with one malloc */
double* allocate_matrix_as_array(int nrows, int ncols) {
  double *arr_A;
  /* Allocate enough raw space */
  arr_A = (double*) malloc(nrows*ncols*sizeof(double));
  return arr_A;
}
...
arr_A[i+ncols+j]
```

If necessary can add a matrix of pointers pointing to the allocated array



Aliasing and restrict

- In C aliasing occurs if two pointers point to the same area of memory.
- Aliasing can severely limit compiler optimisations:
 - difficult to invert the order of the operations, particularly if passed to a function
- The C99 standard introduced the restrict keyword to indicate that aliasing is not possible:

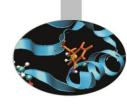
```
void saxpy(int n, float a, float *x, float* restrict y)
```

 In C++ it is assumed that aliasing cannot occur between pointers to different types (strict aliasing).





Aliasing and Restrict /2

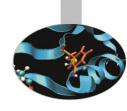


- FORTRAN assumes that the arguments of a procedure cannot point to the same area of memory
 - except for arrays where in any case the indices allow a correct behaviour
 - or for pointers which are used anyway as arguments
 - one reason why FORTRAN optimises better than C!
- It is possible to configure the aliasing options at compile time
 - GNU (solo strict-aliasing): -fstrict-aliasing
 - Intel (complete elimination): -fno-alias
 - IBM (no overlap per array): -qalias=noaryovrlp





Input/Output

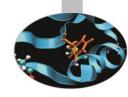


- I/O is performed by the operating system and:
 - results in a system call
 - empties the pipeline
 - destroys the coherence of data in the cache
 - is very slow
- Rule 1: Do not mix intensive computing with I/O
- Rule 2: read/write data in blocks, not a few bytes at a time (the optimum block size depends on filesystem)





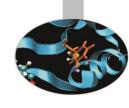
Fortran I/O examples



```
do k=1,n; do j=1,n; do i=1,n
write(69,*) a(i,j,k)
                                              ! formattated
enddo ; enddo ; enddo
do k=1,n; do j=1,n; do i=1,n
write (69) a (i,j,k)
                                              ! binary
enddo ; enddo ; enddo
do k=1,n; do j=1,n
write (69) (a(i,j,k),i=1,n)
                                              ! columns
enddo ; enddo
do k=1,n
write (69) ((a(i,j,k),i=1),n,j=1,n)
                                              ! matrices
enddo
write (69) (((a(i,j,k),i=1,n),j=1,n),k=1,n)
                                              ! block
write(69) a
                                              ! dump
```



FORTRAN I/O performances

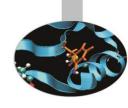


Option	Seconds	Kbytes
Formatted	81.6	419430
Binary	81.1	419430
Columns	60.1	268435
Matrix	0.66	134742
Block	0.94	134219
Dump	0.66	134217





I/O Summary



- Reading/writing formatted data is slow.
- Better to read/write binary data.
- Read/write in blocks.
- Choose the most efficient filesystem available.
- Note that although writing is generally buffered, the impact on performance can be significant.
- For parallel programs:
 - avoid having every task perform read/writes
 - use instead MPI I/O, NetCDF or HDF5, etc.



Summary



- Most programmers optimise their codes by simply increasing the optimisation level during the compilation but with complex programs the compiler normally needs help. Code optimisation is a partnership between programmer and compiler.
- Many serial optimisations, regardless of language (C, Fortran,..), work towards optimal cache and vector performance – particularly essential for hybrid HPC architectures (e.g. GPU, Xeon PHI).
- Since most optimisations work on arrays always bear in mind how arrays are stored in memory (i.e. row-order or column order).