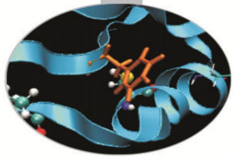
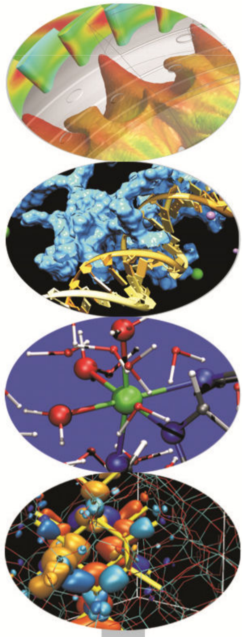


Compilers and Optimisation



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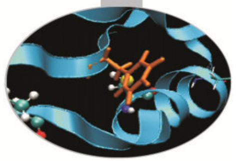
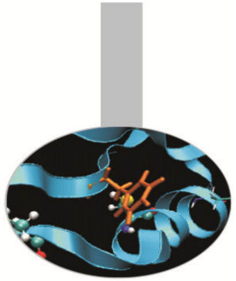
SCAI, Cineca

Contents



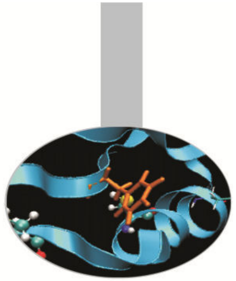
- Introduction
- Optimisation levels
- Specific hardware optimisations
  - IBM
  - Intel
- Typical optimisations
  - Loops
- Compilation and optimisation examples
  - Simple compilation, compilation and linking, static and shared libraries

Introduction



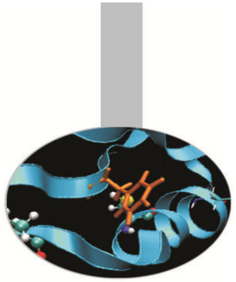
- The hardware components of modern supercomputers are capable providing substantial computing power
- To obtain high performing applications we require:
  - Efficient programming
  - A good understanding of the compilers and how that optimize code for the underlying hardware
  - Tools such as profilers,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

The compiler



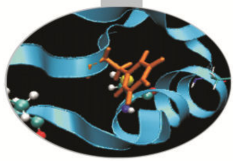
- There are many compilers available and for all computer operating systems (e.g. Linux, Windows or Macintosh).
- As well as free compilers from the GNU project there are also various commercial compilers (e.g. Portland or Intel)
- Some compilers are provided with the hardware (IBM XL for Fermi)

Compilers and interpreters



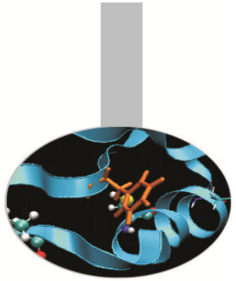
- Interpreted languages
  - The code is “translated” statement-by-statement during the execution
  - Easier on the programmer, modifications can be made quickly but optimisations between different statements (almost) impossible
  - Used for scripting languages (bash, Perl, PHP, ..)
- Compiled languages
  - 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?



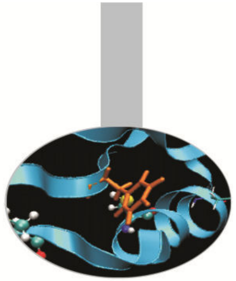
- Translates source code into machine code, if no syntax errors found. Warnings for potential semantic problems.
- Can attempt to optimise the code. Optimisations can be:
  - Language dependent or independent
  - Hardware dependent (e.g. CPU, memory, cache)
- Compilers are very sophisticated software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

Pre-processing, compiling and linking



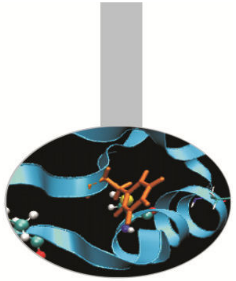
- "Compiling" a program is actually a three stage process:
  1. Pre-processing to replace MACROs (`#define`), code insertions (`#include`), code selections (`#ifdef, #if`). Originally C/C++ but also used in FORTRAN .
  2. Compilation of the source code into object files – organised collections of symbols 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 ?



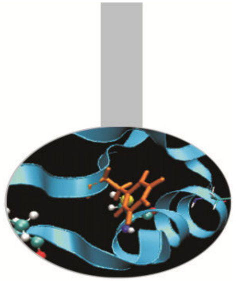
- Common compiler suites include:
  - GNU (gcc, gfortran,...)
  - Intel (icc, icpc, icc)
  - IBM (xlf, xlc, xlC)
  - Portland (pgf90, pgcc, pgCC)
  - LLVM (Clang)
- If I have a choice, which one ?
  - Various things to consider. For performance vendor-specific (e.g xlf on BG/Q, Intel on Intel CPUs) but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

What does the compiler do?

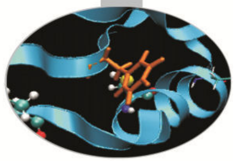


- The compiler can perform many optimisations including:
  - Register allocation
  - Dead and redundant code removal
  - Common subexpression elimination (CSE)
  - Strength reduction (e.g. replacing an exponentiation within a loop with a multiplication)
  - Inlining
  - Loop optimisations such as index 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
  - Unrolling/Merging/Blocking with
    - Calls to functions or subroutines
    - I/O statements or calls within the code
  - Function in-lining if not explicitly indicated by the programmer
  - Optimize variables with values known only at run-time

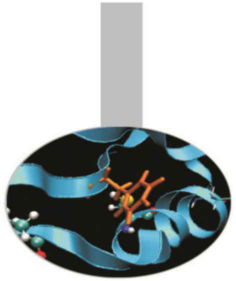


Optimisation options - Intel

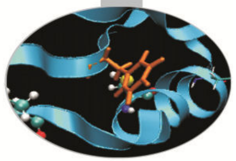
```
icc (or ifort) -O3
```

- 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)

Optimisation options



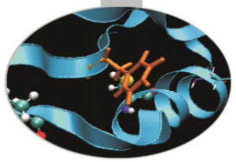
- Compilers give the possibility of specifying optimisation options at compile time, together with the other options.
- These are either general optimisation levels or specific flags related to the underlying hardware.
- Some options can greatly increase the compilation time so one reason for starting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



Optimisation levels –common to all HPC compilers

- -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.

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



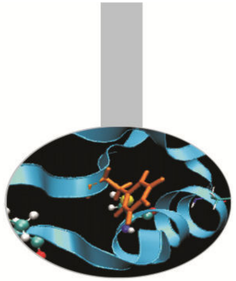
- Example: matrix-matrix multiplication (1024x1024), double precision, FORTRAN.
- Two systems:
  - FERMI: (IBM BG/Q Power A2, 1.6Ghz)
  - PLX: (Xeon Westmere CPUs, 2.4 Ghz)

FERMI xlf

Option	Seconds	MFlops
-O0	65.78	32.6
-O2	7.13	301
-O3	0.78	2735
-O4	55.52	38.7
-O5	0.65	3311

PLX -ifort

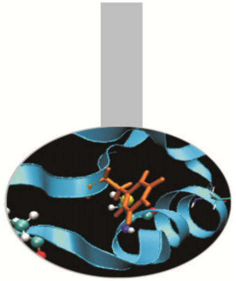
Option	Seconds	MFlops
-O0	8.94	240
-O2	1.41	1514
-O3	0.72	2955
-O4	0.33	6392
-O5	0.32	6623



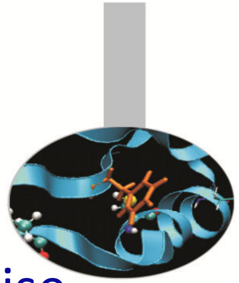
Can I just leave it to the compiler to optimise my code ?

- 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.



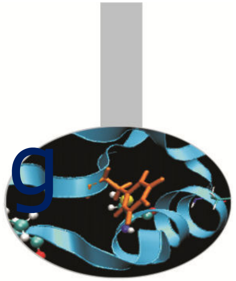
Loop optimisations

- 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

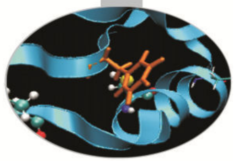


For simple loops, the compiler optimises well

```
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

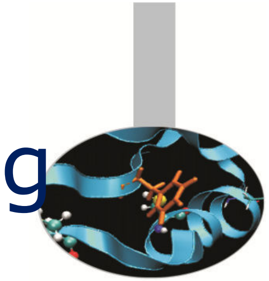


- For more complex, nested loops optimised performances may differ.
- Important to understand the cache mechanism!

```
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;
};
```

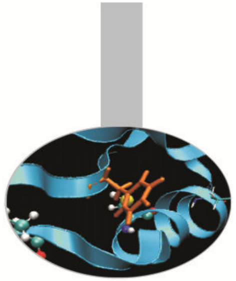
If not then performance is slow. By adding loops, can reduce data held such that it fits into cache.

```
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;
          };
```

B=blocking factor

a[i] = b[i] + c[i];

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];
```

```
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];

}
```

in some cases can eliminate a loop altogether

Loop optimisations – loop fusion

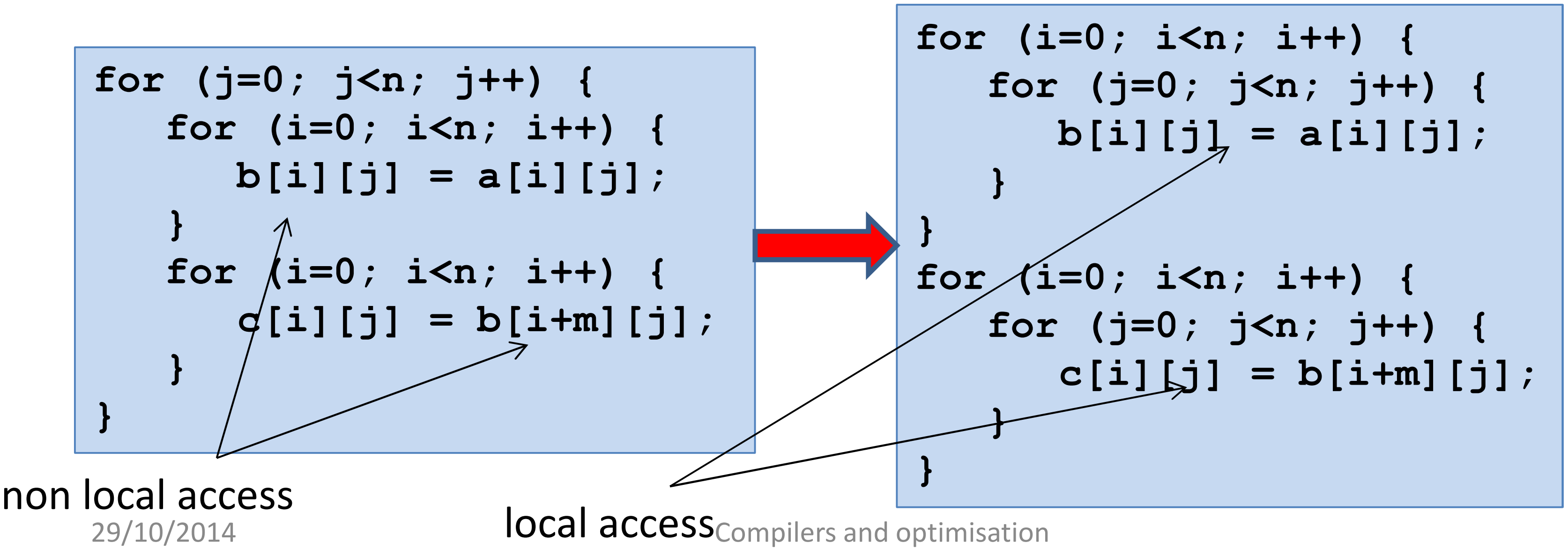
- A loop transformation which replaces multiple loops with a single one (to avoid loop overheads and aid cache use).
- Possible when two loops iterate over the same range and do not reference each other’s data. (unless “loop peeling” is used)
- Doesn’t always improve performance – sometimes cache is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

```
/* 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
```

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.



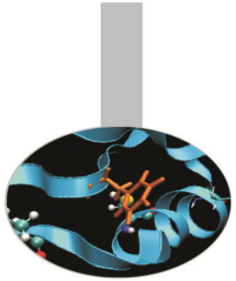
```
for (j=0; j<n; j++) {
   for (i=0; i<n; i++) {
      b[i][j] = a[i][j];
   }
   for (i=0; i<n; i++) {
      c[i][j] = b[i+m][j];
   }
}
```

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

non local access

local access

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

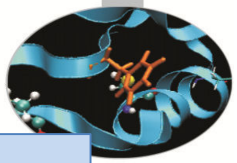


- Depends on access patterns, but for vectorised C/C++ usually preferable to have SoA rather than AoS since array elements are contiguous in memory.
- SoA also usually uses less memory because of data alignment.

```
// 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 node {
   float x,y,z;
   int n;
};

struct node NODES[N];

for (i=0;i<N;i++) {
   NODES[i].x=1;
   NODES[i].y=1;
   NODES[i].z=1;
}
for (i=0; i<N; i++) {
   x=NODES[i].x;
   y=NODES[i].y;
   z=NODES[i].z;
   sum+=sqrtf(x*x+y*y+z*z);
```

```
// Struct of Arrays
struct node {
   float x[N];

struct node NODES;

for (i=0;i<N;i++) {
   NODES.x[i]=1;
   NODES.y[i]=1;
   NODES.z[i]=1;
}
for (i=0; i<N; i++) {
   x=NODES.x[i];
   y=NODES.y[i];
```

```
icc -O2 -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
```

```
icc -O2 -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
```

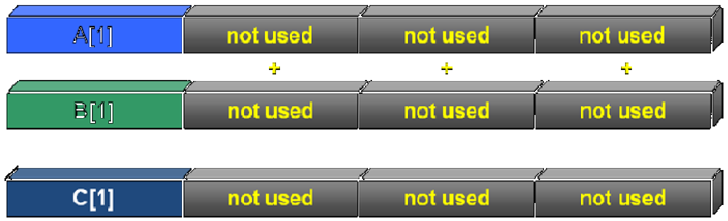
Vectorisation

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

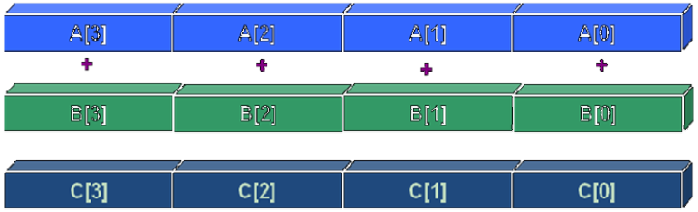
```
c(0) = a(0) + b(0)
c(1) = a(1) + b(1)
c(2) = a(2) + b(2)
c(3) = a(3) + b(3)
```

non vectorised

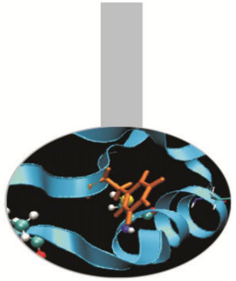
e.g. 3 x 32-bit unused integers



vectorised

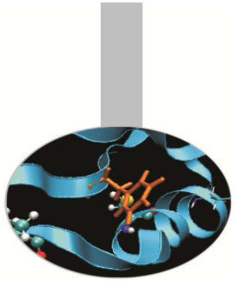


Vectorisation evolution



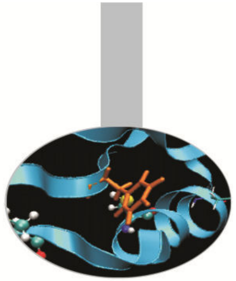
- SSE: 128 bit registers (intel Core - AMD Opteron)
  - 4 floating/integer operations in single precision
  - 2 floating/integer operations in double precision
- AVX: 256 bit registers (intel Sandy Bridge - AMD Bulldozer)
  - 8 floating/integer operations in single precision
  - 4 floating/integer operations 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

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



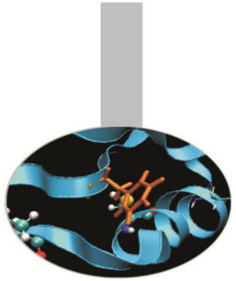
- Different algorithms performing the same task can behave differently wrt vectorisation.
  - Gauss-Seidel: dipendency between iterations, not vectorisable.

```
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]);
```

  - Jacobi: no dipendency, 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];
```

Helping the vectoriser



- Some “coding tricks” can block vectorisation:
  - vectorisable

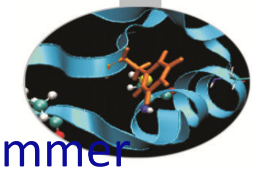
```
for( i = 0; i < n-1; ++i ){
        b[i] = a[i] + a[i+1];
}
```

  - 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;
}
```

- 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

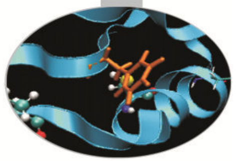
Helping the vectoriser



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

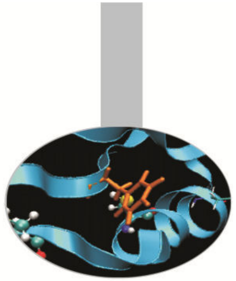
```
do k = 1,n

!DIR$ simd
   do i = 1,l
   ...
    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
    a06(i,k,inew) = x06 - omega*(x06-e06)
```

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

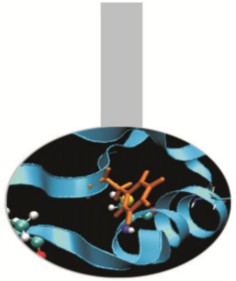
  ```
  A = B+C+D
  E = B+F+C
  ```

  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



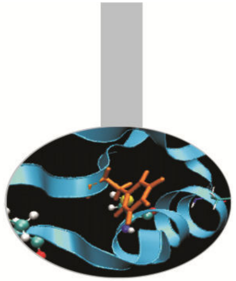
- By altering the order of the calls the compiler doesn’t know if the result is affected (possible side-effects)
- 5 function calls, 5 products

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

- 4 function calls, 4 products (1 temporary variable)

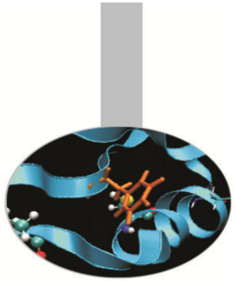
```
temp=r*sin(a)
x=temp*cos(b);
y=temp*sin(b);
z=r*cos(a);
```

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

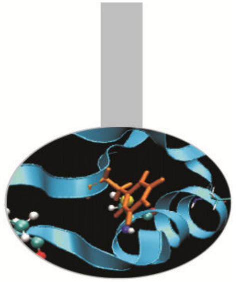


- Compiler dependent. Intel provides various useful options:

```
-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

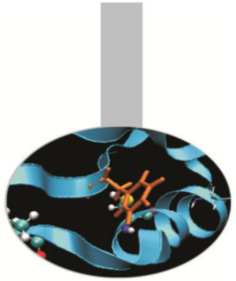


- Static allocation in principle can help the compiler optimise by providing more information. But
  - the code becomes more rigid
  - in parallel computing dynamic allocation is very useful

```
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))
```

Static and Dynamic Allocation



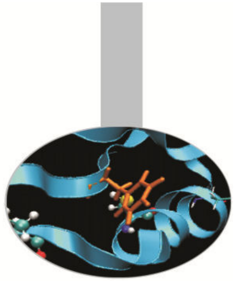
- For recent compilers, performances are often similar for static and dynamic allocations.
  - e.g. matrix-matrix multiplication

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
ulimit -s unlimited
```

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;
}
```

Dynamic array allocation in C/2

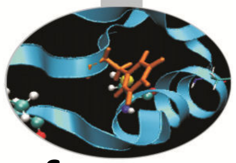
- Better to allocate a linear (1D array) and use it as matrix (*index linearisation*).

```
/* 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

```
/* Allocate a double matrix with one malloc */
double** allocate_matrix(int nrows, int ncols, double* arr_A) {
double **A;
/* Prepare pointers for each matrix row */
A = new double*[nrows];
/* Initialize the pointers */
for (int ii=0; ii<nrows; ++ii) {
A[ii] = &(arr_A[ii*ncols]);
}
return A;
}
```

Aliasing and restrict

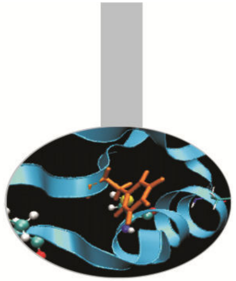


- In C *aliasing* occurs if two pointers point to the same area of memory.
- Aliasing can severely limit compiler optimisations:
  - difficult to invert the order of the operations, particularly if passed to a function
- The C99 standard introduced the `restrict` keyword to indicate that aliasing is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

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

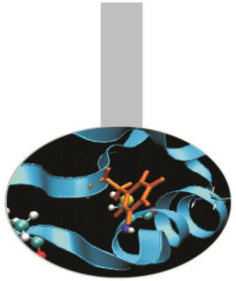
- In C++ it is assumed that aliasing cannot occur between pointers to different types (strict aliasing).

Aliasing and Restrict /2



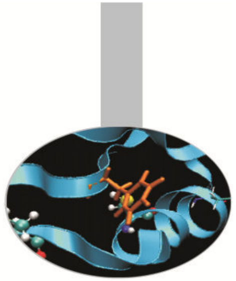
- FORTRAN assumes that the arguments of a procedure cannot point to the same area of memory
  - except for arrays where in any case the indices allow a correct behaviour
  - or for pointers which are used anyway as arguments
  - one reason why FORTRAN optimises better than C!
- It is possible to configure 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

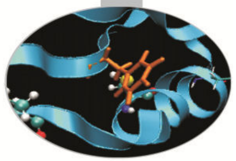


- I/O is performed by the operating system and:
  - results in a system call
  - empties the pipeline
  - destroys the coherence of data in the cache
  - is very slow
- Rule 1: Do not mix intensive computing with I/O
- Rule 2: read/write data in blocks, not a few bytes at a time (the optimum block size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

Fortran I/O examples



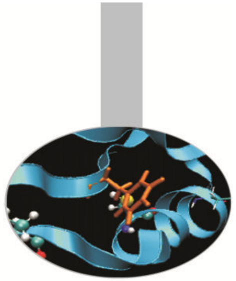
```
do k=1,n ; do j=1,n ; do i=1,n
write(69,*) a(i,j,k)                    ! formattated
enddo ; enddo ; enddo
do k=1,n ; do j=1,n ; do i=1,n
write(69) a(i,j,k)                      ! binary
enddo ; enddo ; enddo
do k=1,n ; do j=1,n
write(69) (a(i,j,k),i=1,n)              ! columns
enddo ; enddo
do k=1,n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

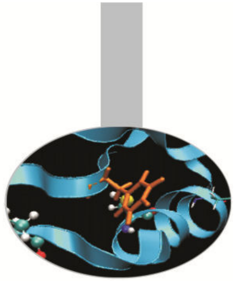
Option	Seconds	Kbytes
Formatted	81.6	419430
Binary	81.1	419430
Columns	60.1	268435
Matrix	0.66	134742
Block	0.94	134219
Dump	0.66	134217

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.
- 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).