Tips and tricks for optimization of Fortran codes

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In this short report, we have shown the simple optimization tips and tricks which can be used in general scientific programming with focus on Fortran.

I.

Compiler Options;

- Substantial gain can be easily obtained by playing with compiler options
- Optimization options are a must. The first and second level of optimization will rarely give no benefits!
- Optimization options can range from -O1 to -O5 with some compilers. -O3 to -O5 might lead to slower code, so try them independently on each subroutine.
- Always check your results when trying optimization options.
- Compiler options might include hardware specifics such as accessing vector units for example.

Intel Fortran and C compiler Options:
ifort, ifc and icc
    -O0 -O1 -O2 -O3 -ip -xW -tpp7(for P4) -ip ...

Vectorizing of DO loop; a DO loop can be vectorized when each array calculation is independent of another one

```
DO ix=1, Nx
    A(ix)=B(ix)×C(ix)+D(ix)
END DO
```

→

```
A=B×C+D
```

```
DO i=1, 1000
    DO j=1, 1000
        DO k=1, 500
            A(i,j,k) = X(i) × Y(j)
                       +Z(i,j,k)
                       +2.0/X(i)**2
        END DO
    END DO
END DO
```

→

```
DO j=1, 1000
    DO k=1, 500
        A(:,j,k) = X × Y(j)
                   +Z(:,j,k)
                   +2.0/X**2
    END DO
END DO
```

2000 Millions of operations **2 Millions of operations**

SUM function; summation by using SUM function instead of DO Loops

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```
Sumx=0
DO ix=1, Nx
    Sumx=Sumx+W(ix)× F(ix)
END DO
```

→

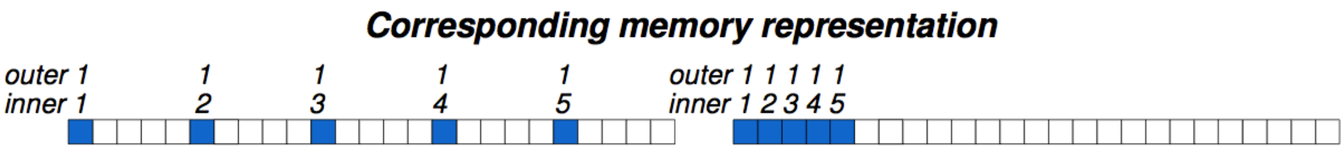
```
Sumx=SUM(W×F)
```

Array Considerations; try to minimize the memory jumps, they could be very costly because of cache and TLB misses

```
DO i=1, Ni
    DO j=1, Nj
        A(i,j) = ···
    END DO
END DO
```

→

```
DO j=1, Nj
    DO i=1, Ni
        A(i,j) = ···
    END DO
END DO
```



Minimizing the number of operations; one of the first thing for optimization is reducing the number of unnecessary operations performed by the CPU!

```
DO k=1, 10
    DO j=1, 5000
        DO i=1, 5000
            A(i,j,k) = 3.0 × m × D(k)+
                       C(j) × 23.5−
                       B(i)
        END DO
    END DO
END DO
```

→

```
DO k=1, 10
    Dtmp(k) = 3.0 × m×D(k)
    DO j=1, 5000
        Ctmp(j) = C(j) × 23.5
        DO i=1, 5000
            A(i,j,k) = Dtmp(k)+
                       Ctmp(j)−
                       B(i)
        END DO
    END DO
END DO
```

1250 Millions of operations **500 Millions of operations**

Complex Numbers; look for operations on complex numbers that have Imaginary or Real part equal to zero. This is again a question of minimizing the number of operations.

```
! Real part of A elements = 0
COMPLEX*16 A(1000,1000), B, C(1000,1000)

DO j=1, 1000
    DO i=1, 1000
        C(i,j) = A(i,j) × B
    END DO
END DO
```

→

```
REAL*8        AI(1000,1000)
COMPLEX*16 B, C(1000,1000)

DO j=1, 1000
    DO i=1, 1000
        C(i,j) = ( -IMAG(B) × AI(i,j),
                   AI(i,j) × REAL(B) )
    END DO
END DO
```

6 Millions of operations

2 Millions of operations

Loop Overhead and Objects declarations and instanciations; in Object-Oriented Languages AVOID objects declarations and instanciations within the most inner loops

```
DO j=1, 1000000
    DO i=1, 100000
        DO k=1, 2
            A(i,j,k) = B(i,j) + C(k)
        END DO
    END DO
END DO
```

→

```
DO j=1, 1000000
    DO i=1, 100000
        A(i,j,1) = B(i,j) + C(1)
        A(i,j,2) = B(i,j) + C(2)
    END DO
END DO
```

Function Call Overhead;

```
DO k=1, 10000
    DO j=1, 10000
        DO i=1, 5000
            A(i,j,k) = F1( C(i), B(j), k )
        END DO
    END DO
END DO

FUNCTION F1(x,y,m)
  REAL*8 x,y,tmp
  INTEGER m
  tmp=x*m - y
  RETURN tmp
END FUNCTION
```

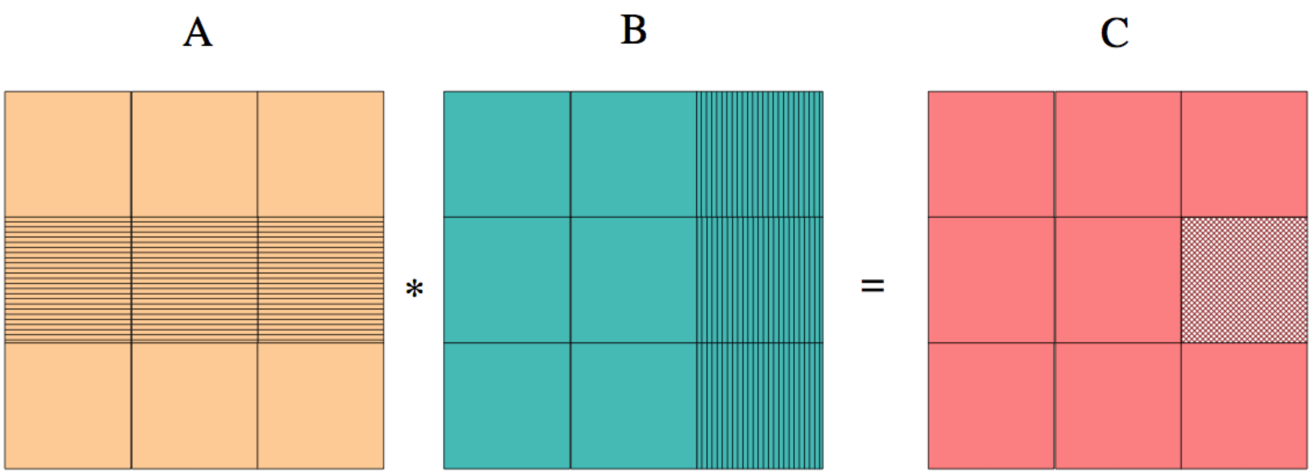
→

```
DO k=1, 10000
    DO j=1, 10000
        DO i=1, 5000
            A(i,j,k) = C(i) * k - B(j)
        END DO
    END DO
END DO
```

Blocking; Blocking is used to reduce cache and TLB misses in nested Matrix operations. The idea is to process as much as possible the data that is brought in the cache.

```
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
```

```
DO ib=1, N, bsize
    DO jb=1, N, bsize
        DO kb=1, N, bsize
            DO i=ib, min(N,ib+bsize-1)
                DO j=jb,min(N,jb+bsize-1)
                    DO k=kb,min(N,kb+bsize-1)
                        C(i,j) = C(i,j)
                               +A(i,k)*B(k,j)
                    END DO
                END DO
            END DO
        END DO
    END DO
END DO
```




```
C(i,j)=C(i,j)+A(i,k)*B(k,j)
```

Loop Fusion; The main advantage of Loop Fusion is the reduction of cache misses when the same array is used in both loops. It also reduces loop overhead and allow a better control of multiple instructions in a single cycle, when hardware allows it (2 FMA or 2 vector operations for example).

```
DO i=1, 10000
    A = A + X(i) + 2.0*Z(i)
END DO

DO i=1, 10000
    B = 3.0×X(i) - 5.0
END DO
```

```
DO i=1, 10000
    A = A + X(i) + 2.0*Z(i)
    B = 3.0×X(i) - 5.0
END DO
```

Loop Unrolling; the main advantage of Loop Unrolling is to reduce or eliminate data dependencies in loops. This is particularly useful when using an architecture with 2 FMA Units (IBM Power3-4) or a Vector unit (SSE2 extensions)

```
DO i=1, 1000
      A = A + X(i) × Y(i)
END DO
```

→

```
DO i=1, 1000, 4
      A = A + X(i) × Y(i)
            +X(i + 1) × Y(i + 1)
            +X(i + 2) × Y(i + 2)
            +X(i + 3) × Y(i + 3)
END DO
```

Sum Reductions; sum reductions is another way of reducing or eliminating data dependencies in loops. It is more explicit than the Loop Unrolling method.

```
DO i=1, 1000
      A = A + X(i) × Y(i)
END DO
```

→

```
DO i=1, 1000, 4
      A1 = A1 + X(i) × Y(i)
      A2 = A2 + X(i + 1) × Y(i + 1)
      A3 = A3 + X(i + 2) × Y(i + 2)
      A4 = A4 + X(i + 3) × Y(i + 3)
END DO
A = A1 + A2 + A3 + A4
```

Replace divisions by multiplications; Contrary to Floating Point multiplications or additions or subtractions, divisions are very costly in terms of clock cycles.

1 multiplication = 1 cycle
1 division = 14-20 cycles

```
DO j=1, 10000
      DO i=1, 10000
            A(i, j) = (B(i) − C(j))/D
      END DO
END DO
```

→

```
D = 1.0/D
DO j=1, 10000
      DO i=1, 10000
            A(i, j) = (B(i) − C(j)) × D
      END DO
END DO
```

Repeated multiplications for exponentials; exponentiation with a small exponent should be done manually. Like divisions exponential operations use many cycles.

```
A = B ∗ ∗3.0
```

→

```
tmpc = B ∗ B
A = tmpc ∗ B
```

Breaking Interpolations; the multi-dimensional interpolations should be considered as few one dimensional interpolations

Branching (proper use of IFs); try to minimize as much as possible the use of IFs within the inner loops. The CPU will first assume a YES when it encounters a IF statement while filling up the instruction pipline.