# **MAQAO Hands-on exercises LRZ Cluster**

LProf: lightweight generic profiler

LProf/MPI: Lightweight MPI oriented profiler

CQA: code quality analyzer

















#### Setup

#### Copy handson material

> cp /home/hpc/a2c06/lu23bud/LRZ-VIHPSTW21/tools/maqao/MAQAO\_HANDSON\_LRZ.tar.xz \$HOME

#### Untar the archive at the root of your HOME folder

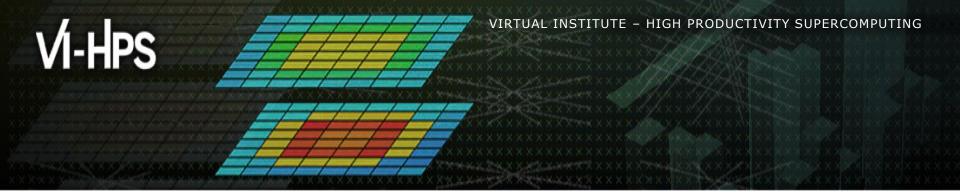
- > cd \$HOME
- > tar xf MAQAO\_HANDSON\_LRZ.tar.xz
- > cd MAQAO\_HANDSON

Copy MPI GUI

> scp -r MPI\_GUI my\_machine:

Add MAQAO path to your local path

> source ./scripts/env.sh



## MAQAO LProf Hands-on exercises

Jean-Baptiste LE-RESTE





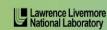
**JÜLICH** 

















#### Setup

Go to the Handson folder

> cd \$HOME/MAQAO\_HANDSON

Locate script and modify it as needed

> vim scripts/lprof\_bt-mz\_ompi.5P.2T.sh

Launch your job

> sbatch scripts/lprof\_bt-mz\_ompi.5P.2T.sh

Visualize the results

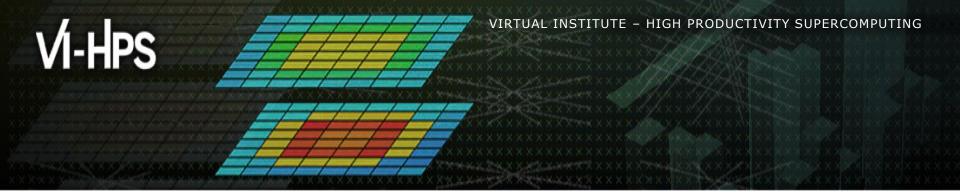
> ./scripts/display.sh (then follow the instructions displayed in the terminal)



#### **Using MAQAO LProf**

A copy of the output is located in output\_examples/LProf folder in case you experience a problem

Now follow live demo/comments



## MAQAO LProfMPI Hands-on exercises

Jean-Baptiste LE-RESTE







Lawrence Livermore
National Laboratory















#### Setup

Go to the Handson folder

> cd \$HOME/MAQAO\_HANDSON

Locate script and modify it as needed

> vim scripts/lprof-mpi\_bt-mz\_intel.5P.2T.sh

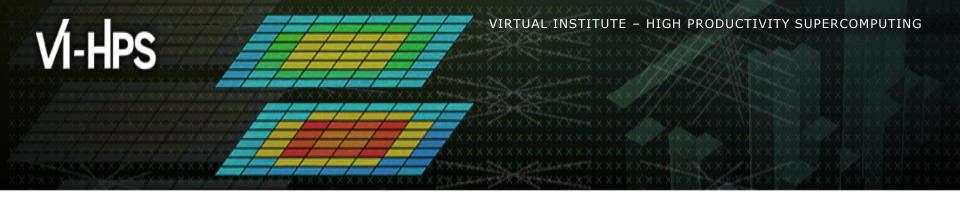
Launch your job

> sbatch scripts/bt-mz\_ompi.5P.2T\_lprof\_mpi.sh

Visualize the results

Copy/Paste the directory ./MPI\_GUI and the file ./results/MPI\_Profile.js locally.

Then open the MPI\_GUI/res/MPI.html and load the MPI\_Profile.js file.



## MAQAO / CQA Hands-on exercises

**Emmanuel OSERET** 





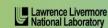
**J**ÜLICH

















#### **Setup for UV2 (Westmere)**

Login uv2

> ssh uv2

Load a recent GCC compiler

> module load gcc/5

Switch to CQA handson folder

> cd \$HOME/MAQAO\_HANDSON/CQA/matmul

#### **Matrix Multiply code**

```
void kernel0 (int n,
              float a[n][n],
              float b[n][n],
              float c[n][n]) {
 int i, j, k;
  for (i=0; i< n; i++)
    for (j=0; j< n; j++) {
      c[i][j] = 0.0f;
      for (k=0; k< n; k++)
        c[i][j] += a[i][k] * b[k][j];
```

"Naïve" dense matrix multiply implementation in C



#### Compiling, running and analyzing kernel0 in -O3

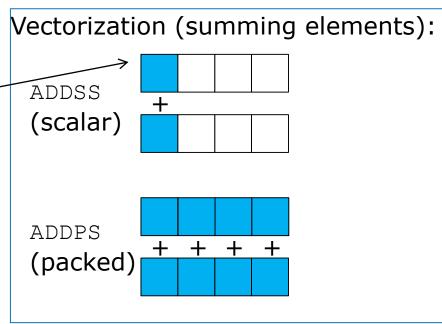
```
> make OPTFLAGS=-03 KERNEL=0
> ./matmul 100 1000
Cycles per FMA: 3.27
> maqao cqa matmul fct-loops=kernel0 [of=html]
```

NB: the usual way to use CQA consists in finding IDs of hot loops with the MAQAO profiler and forwarding them to CQA (loop=17,42...).

To simplify this hands-on, we will bypass profiling and directly requesting CQA to analyze all innermost loops in functions (max 2-3 loops/function for this hands-on).

#### CQA output for kernel0 (from the "gain" confidence level)

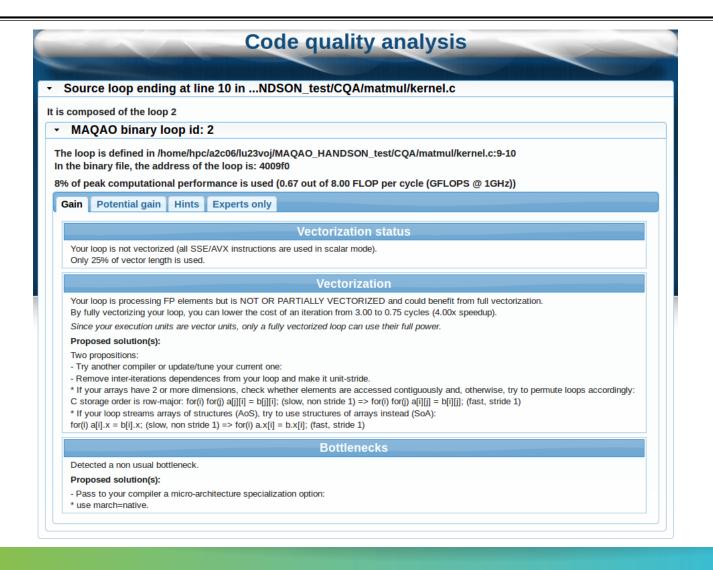
```
Vectorization
(...) By fully vectorizing your loop,
you can lower the cost of an iteration
from 3.00 to 0.75 cycles (4.00x)
speedup). (...)
 - Remove inter-iterations dependences
from your loop and make it unit-
stride.
  * If your arrays have 2 or more
dimensions, check whether elements are
accessed contiguously and, otherwise,
try to permute loops accordingly:
C storage order is row-major: for(i)
a[j][i] = b[j][i]; (slow, non stide 1)
=> for(i) for(j) a[i][j] = b[i][j];
(fast, stride 1)
  * If your loop streams arrays of
structures (AoS), try to use (...) SoA
```



- Accesses are not contiguous => let's permute k and j loops
- ¬■ No structures here...

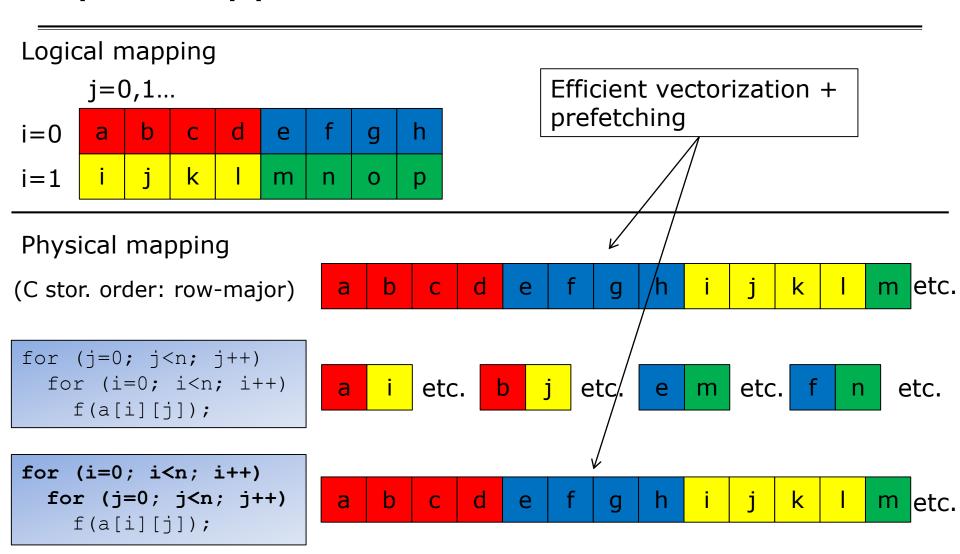


#### CQA output for kernel0 (from the "gain" confidence level)





#### Impact of loop permutation on data access





# Removing inter-iteration dependences and getting stride 1 by permuting loops on j and k

```
void kernell (int n,
              float a[n][n],
              float b[n][n],
              float c[n][n]) {
  int i, j, k;
  for (i=0; i<n; i++) {
    for (j=0; j< n; j++)
      c[i][j] = 0.0f;
    for (k=0; k< n; k++)
      for (j=0; j< n; j++)
        c[i][j] += a[i][k] * b[k][j];
```



#### kernel1: loop interchange

```
> make clean
> make OPTFLAGS=-03 KERNEL=1
> ./matmul 100 1000
Cycles per FMA: 1.03
> maqao cqa matmul fct-loops=kernel1 --confidence-levels=gain,potential,hint
```



#### CQA output for kernel1 (from "gain" and "hint" conf. levels)

Vectorization status

Your loop is fully vectorized...

Vector unaligned load/store instructions

\_\_\_\_\_\_

- Use vector aligned instructions:
- align your arrays on 32 bytes boundaries,
- 2) inform your compiler that your arrays are vector aligned:
- \* use the \_\_builtin\_assume\_aligned built-in

 Let's switch to the next proposal: vector aligned instructions

#### Aligning vector accesses in driver + assuming them in kernel

```
int main (...) {
  (...)
#if KERNEL==2
 puts (« driver.c: Using
posix memalign instead of malloc »);
 posix memalign ((void **) &a, 32,
size in bytes);
 posix memalign ((void **) &b, 32,
size in bytes);
 posix memalign ((void **) &c, 32,
size in bytes);
#else
  a = malloc (size in bytes);
 b = malloc (size in bytes);
  c = malloc (size in bytes);
#endif
  (...)
```

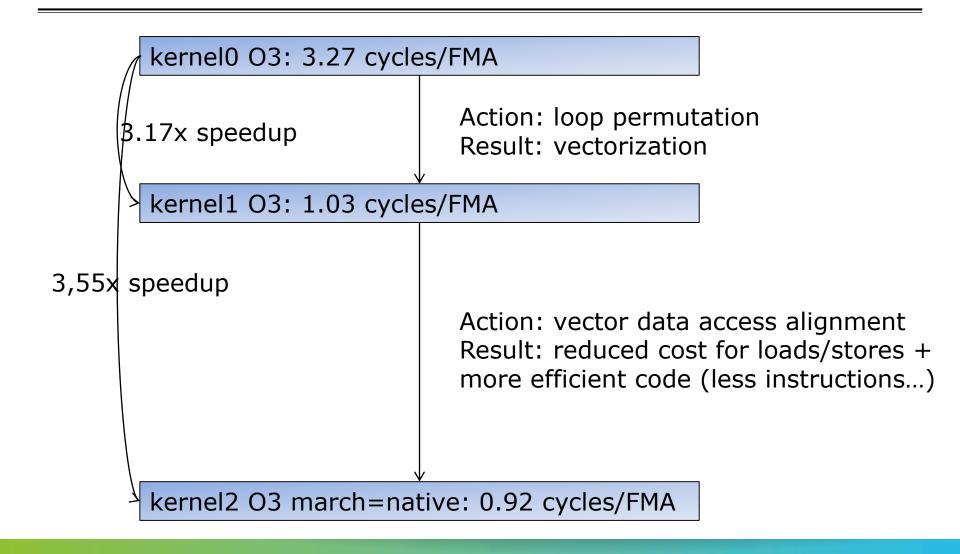
```
void kernel2 (int n,
              float a[n][n],
              float b[n][n],
              float c[n][n]) {
  int i, j, k;
 for (i=0; i<n; i++) {
    float *ci =
 builtin assume aligned (c[i], 32);
    for (j=0; j < n; j++)
      ci[j] = 0.0f;
    for (k=0; k< n; k++) {
      float *bk =
 builtin assume aligned (b[k], 32);
      for (j=0; j < n; j++)
        ci[j] += a[i][k] * bk[j];
```



#### kernel2: assuming aligned vector accesses

```
> make clean
> make OPTFLAGS=-03 KERNEL=2
> ./matmul 100 1000
Cannot call kernel2 on matrices with size%8 != 0 (data non aligned on 32B boundaries)
Aborted
> ./matmul 104 1000
Cycles per FMA: 0.92
```

#### **Summary of optimizations and gains**





#### What if Haswell?

CQA can cross-analyze to another micro-architecture



## Compiling and analyzing kernel0 in -O3

```
> make OPTFLAGS=-03 KERNEL=0
```

> maqao cqa matmul uarch=HASWELL fct-loops=kernel0



#### CQA output for kernel0 (from the "gain" confidence level)

```
Vectorization
-----

(...) By fully vectorizing your loop,
you can lower the cost of an iteration
from 3.00 to 0.38 cycles (8.00x

speedup).(...)

8x instead of 4x
```



## kernel1: loop interchange

- > make clean
- > make OPTFLAGS=-03 KERNEL=1
- > maqao cqa matmul uarch=HASWELL fct-loops=kernel1

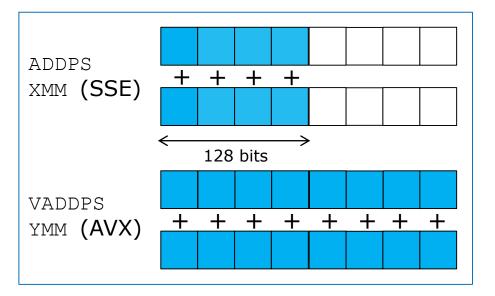
#### **CQA** output for kernel1

Vectorization status Your loop is fully vectorized (...) → ■ Westmere: 100% length... but on 50% vector length. Vectorization - Pass to your compiler a microarchitecture specialization option: \* use march=native Let's add -march=haswell to - Use vector aligned instructions... **OPTFLAGS** FMA Presence of both ADD/SUB and MUL operations. - Pass to your compiler a microarchitecture specialization option... - Try to change order in which ...



#### Impacts of architecture specialization: vectorization and FMA

- Vectorization
  - SSE instructions (SIMD 128 bits) used on a processor supporting AVX ones (SIMD 256 bits)
  - => 50% efficiency loss



- FMA
  - Fused Multiply-Add (A+BC)
  - Intel architectures: supported on MIC/KNC and Xeon starting from Haswell

```
# A = A + BC

VMULPS <B>,<C>,%XMM0
VADDPS <A>,%XMM0,<A>
# can be replaced with
something like:
VFMADD312PS <B>,<C>,<A>
```



#### Kernel1 + -march=native

- > make clean
- > make OPTFLAGS="-03 -march=haswell" KERNEL=1
- > maqao cqa matmul uarch=HASWELL fct-loops=kernel1 --confidencelevels=gain,hint

#### CQA output for kernel1 (using "gain" and "hint" conf. levels)

Vectorization status Your loop is fully vectorized (...) Vector unaligned load/store... - Use vector aligned instructions: 1) align your arrays on 32 bytes boundaries, 2) inform your compiler that your arrays are vector aligned: \* use the builtin assume aligned built-in

Let's switch to the next proposal: vector aligned instructions



## kernel2: assuming aligned vector accesses

```
> make clean
```

```
> make OPTFLAGS="-03 -march=haswell" KERNEL=2
```

#### **Setup for an Haswell node**

CQA can be directly executed on a login node because it uses static analysis

Login lxlogin5/6

> ssh <your\_login>@lxlogin5.lrz.de

Load MAQAO environment

> module load maqao

Load a recent GCC compiler

> module load gcc/5

Switch to CQA handson folder

> cd \$HOME/MAQAO\_HANDSON/CQA/matmul

#### **Matrix Multiply code**

```
void kernel0 (int n,
              float a[n][n],
              float b[n][n],
              float c[n][n]) {
 int i, j, k;
  for (i=0; i< n; i++)
    for (j=0; j< n; j++) {
      c[i][j] = 0.0f;
      for (k=0; k< n; k++)
        c[i][j] += a[i][k] * b[k][j];
```

"Naïve" dense matrix multiply implementation in C



#### Compiling, running and analyzing kernel0 in -O3

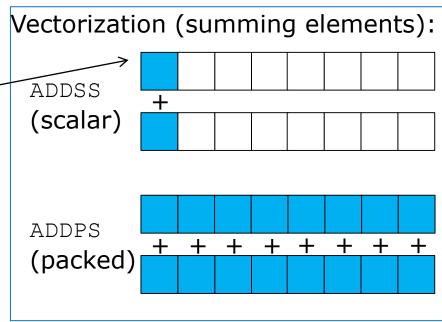
```
> make OPTFLAGS=-03 KERNEL=0
> ./matmul 100 1000
Cycles per FMA: 2.48
> maqao cqa matmul fct-loops=kernel0 [of=html]
```

NB: the usual way to use CQA consists in finding IDs of hot loops with the MAQAO profiler and forwarding them to CQA (loop=17,42...).

To simplify this hands-on, we will bypass profiling and directly requesting CQA to analyze all innermost loops in functions (max 2-3 loops/function for this hands-on).

#### CQA output for kernel0 (from the "gain" confidence level)

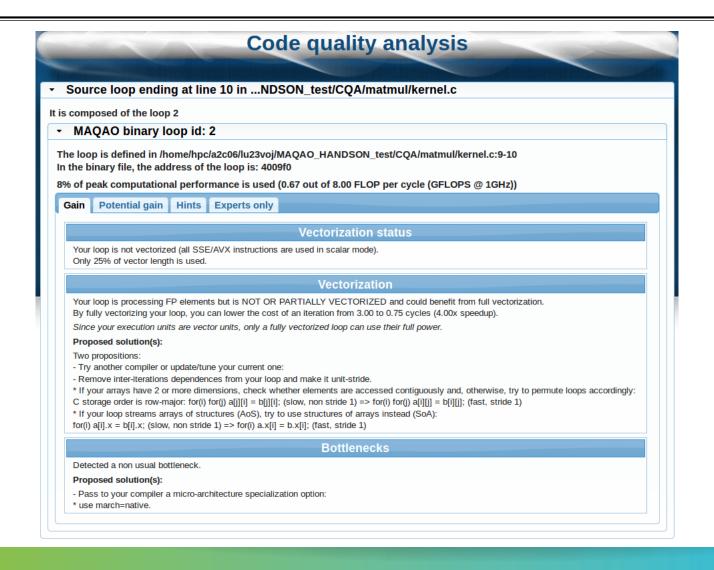
Vectorization (...) By fully vectorizing your loop, you can lower the cost of an iteration from 3.00 to 0.38 cycles (8.00x speedup). (...) - Remove inter-iterations dependences from your loop and make it unitstride. \* If your arrays have 2 or more dimensions, check whether elements are accessed contiguously and, otherwise, try to permute loops accordingly: C storage order is row-major: for(i) a[j][i] = b[j][i]; (slow, non stide 1) => for(i) for(j) a[i][j] = b[i][j]; (fast, stride 1) \* If your loop streams arrays of structures (AoS), try to use (...) SoA



- Accesses are not contiguous => let's permute k and j loops
- ¬■ No structures here...

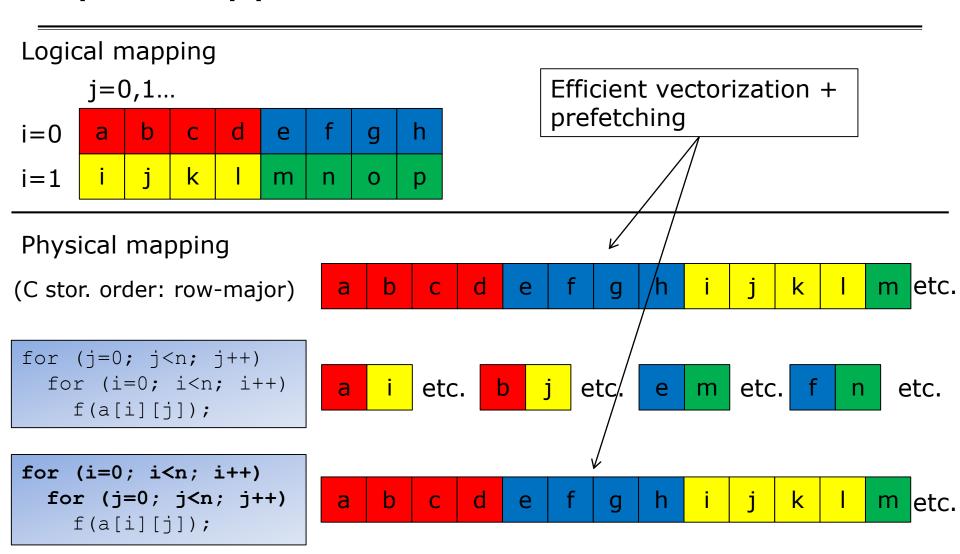


#### CQA output for kernel0 (from the "gain" confidence level)





#### Impact of loop permutation on data access





# Removing inter-iteration dependences and getting stride 1 by permuting loops on j and k

```
void kernell (int n,
              float a[n][n],
              float b[n][n],
              float c[n][n]) {
  int i, j, k;
  for (i=0; i<n; i++) {
    for (j=0; j< n; j++)
      c[i][j] = 0.0f;
    for (k=0; k< n; k++)
      for (j=0; j< n; j++)
        c[i][j] += a[i][k] * b[k][j];
```



### **Kernel1: loop interchange**

```
> make clean
> make OPTFLAGS=-03 KERNEL=1
> ./matmul 100 1000
Cycles per FMA: 0.65
> maqao cqa matmul fct-loops=kernel1
```

# **CQA** output for kernel1

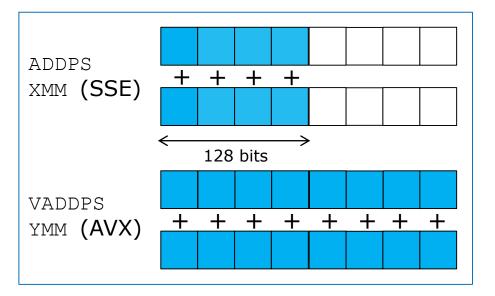
Vectorization status Your loop is fully vectorized (...) but on 50% vector length. Vectorization - Pass to your compiler a microarchitecture specialization option: \* use march=native - Use vector aligned instructions... FMA Presence of both ADD/SUB and MUL operations. - Pass to your compiler a microarchitecture specialization option... - Try to change order in which ...

Let's add -march=native to OPTFLAGS



### Impacts of architecture specialization: vectorization and FMA

- Vectorization
  - SSE instructions (SIMD 128 bits) used on a processor supporting AVX ones (SIMD 256 bits)
  - => 50% efficiency loss



- FMA
  - Fused Multiply-Add (A+BC)
  - Intel architectures: supported on MIC/KNC and Xeon starting from Haswell (hornet)

```
# A = A + BC

VMULPS <B>,<C>,%XMM0
VADDPS <A>,%XMM0,<A>
# can be replaced with
something like:
VFMADD312PS <B>,<C>,<A>
```

### Kernel1 + -march=native

```
> make clean
> make OPTFLAGS="-03 -march=native" KERNEL=1
> ./matmul 100 1000
Cycles per FMA: 0.47
> maqao cqa matmul fct-loops=kernel1 --confidence-levels=gain,hint
```

### CQA output for kernel1 (using "gain" and "hint" conf. levels)

Vectorization status Your loop is fully vectorized (...) Vector unaligned load/store... - Use vector aligned instructions: 1) align your arrays on 32 bytes boundaries, 2) inform your compiler that your arrays are vector aligned: \* use the builtin assume aligned built-in

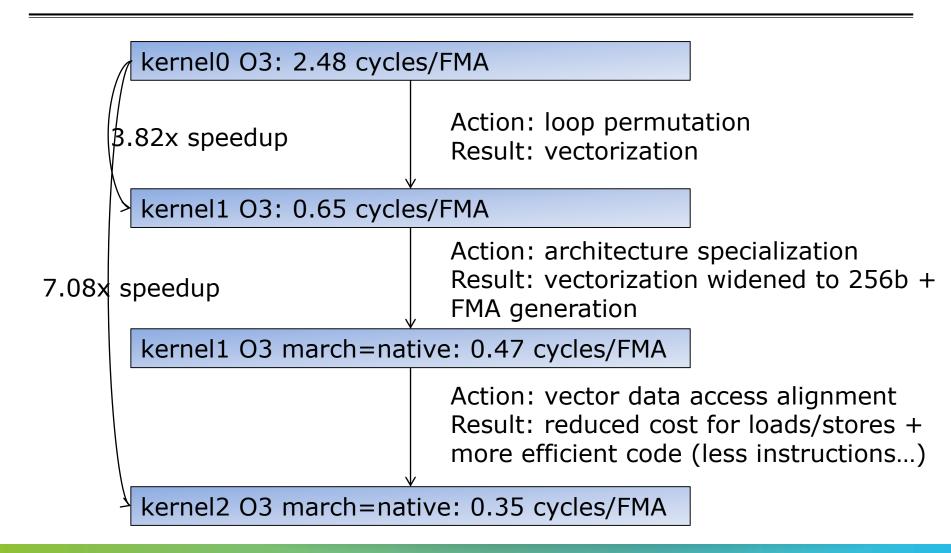
Let's switch to the next proposal: vector aligned instructions



### kernel2: assuming aligned vector accesses

```
> make clean
> make OPTFLAGS="-03 -march=native" KERNEL=2
> ./matmul 100 1000
Cannot call kernel2 on matrices with size%8 != 0 (data non aligned on 32B boundaries)
Aborted
> ./matmul 104 1000
Cycles per FMA: 0.35
```

### **Summary of optimizations and gains**





### **Hydro example**

Switch to the other CQA handson folder

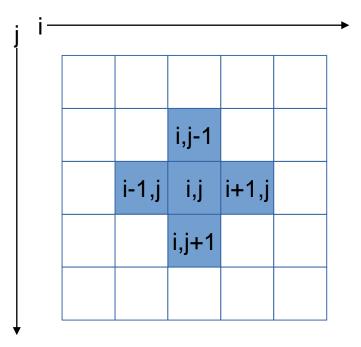
> cd \$HOME/MAQAO\_HANDSON/CQA/hydro

### **Hydro code**

```
int build index (int i, int j, int grid size)
 return (i + (grid size + 2) * j);
void linearSolver0 (...) {
 int i, j, k;
 for (k=0; k<20; k++)
    for (i=1; i<=grid size; i++)
      for (j=1; j<=grid size; j++)</pre>
        x[build index(i, j, grid size)] =
  (a * ( x[build index(i-1, j, grid size)] +
         x[build index(i+1, j, grid size)] +
         x[build index(i, j-1, grid size)] +
         x[build index(i, j+1, grid size)]
       ) + x0[build index(i, j, grid size)]
  ) / c;
```

Iterative linear system solver using the Gauss-Siedel relaxation technique.

« Stencil » code





### Compiling, running and analyzing kernel0 (icc -O3 -xHost)

```
> make KERNEL=0
> ./hydro 250 10 # 1st param: grid size and 2nd param: repet nb
Cycles per element for solvers: 2064.14
> magao lprof xp=sx -- ./hydro 250 10
> magao lprof xp=sx -dl | head
Loop ID
             Function Name
                                              Leve 1
                                                        Time (%)
                              Source Info
142
           project
                            103,105@kernel.c
                                                        28.29
                                             Innermost
           c densitySolver
  54
                          | 103,105@kernel.c
                                            Innermost
                                                        23.03
           c velocitySolver
                          | 103,105@kernel.c
  94
                                            Innermost
                                                        21.71
                          | 103,105@kernel.c
           c velocitySolver
  87
                                            Innermost
                                                       19.08
           project
                            371,374@kernel.c
  140
                                            Innermost
                                                       1.32
> magao cga hydro loop=142
```

In this application the kernel routine, linearSolver, were inlined in caller functions. Moreover, there is here direct mapping between source and binary loop. Consequently the 4 highlighted loops are identical and only one need analysis.

### CQA output for kernel0 (from the "gain" confidence level)

#### Bottlenecks

\_\_\_\_\_

The divide/square root unit is a bottleneck.

By removing all these bottlenecks, you can lower the cost of an iteration from 7.00 to 5.00 cycles (1.40x speedup).

Try to reduce the number of division or square root instructions.

If denominator is constant over iterations, use reciprocal (replace x/y with x\*(1/y)). Check precision impact. This will be done by your compiler with no-prec-div or Ofast.

Cost of a division (about 10-50 cycles) is much higher than for a addition or a multiplication (typically 1 cycle per instruction), especially on double precision elements and on older processors

### Removing (hoisting) division

```
int build index (int i, int j, int grid size)
  return (i + (grid size + 2) * j);
void linearSolver0 (...) {
  int i, j, k;
  const float inv c = 1.0f / c;
  for (k=0; k<20; k++)
    for (i=1; i<=grid size; i*
      for (j=1; j<=grid size; j++)
        x[build index(i, j, grid size)] =
  (a * (x[build index(i-1, j, grid size)] +
         x[build index(i+1, j, grid size)] +
         x[build index(i, j-1, grid size)] +
         x[build index(i, j+1, grid size)]
       ) + x0[build index(i, j, grid size)]
     inv c;
```

Dividing by c is equivalent to multiplying by (1/c). Since c is constant in the loop, the divideby-c operation was hoisted out of the loop and replaced by a multiply inside it

Remark: in some cases applying this optimization can change numerical results (due to rounding). That is why it is not applied by default by compilers.

On this example, no difference when comparing 6 first digits of the decimal part



### kernel1: division removal

```
> make clean
> make KERNEL=1
> ./hydro 250 10
Cycles per element for solvers: 1824.16
> maqao lprof xp=sx2 -- ./hydro 250 50
> maqao lprof xp=sx2 -dl | head
(output similar to KERNEL=0, with same loop Ids)
> maqao cqa loop=142
```

### **CQA** output for kernel1

Composition and unrolling

It is composed of the loop 142 and is not unrolled or unrolled with no peel/tail loop.

The analysis will be displayed for the requested loops: 142

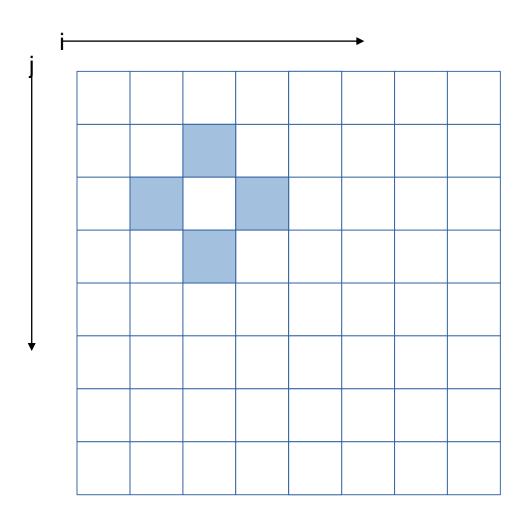
Unroll opportunity

Loop is potentially data access bound.

Unroll your loop if trip count is significantly higher than target unroll factor and if some data references are common to consecutive iterations...

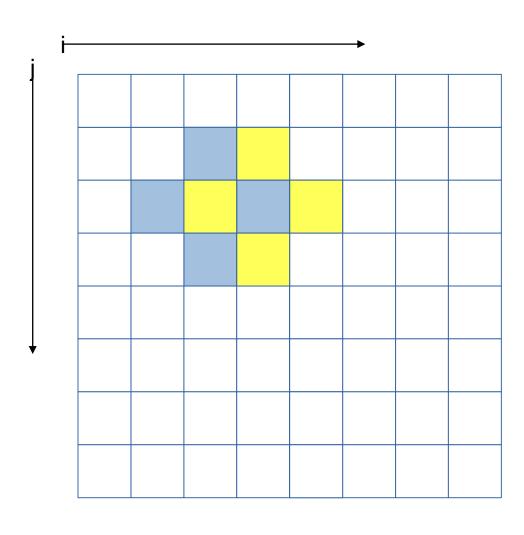
Unrolling is generally a good deal:
fast to apply and often provides
gain. Let's try to reuse data
references through unrolling





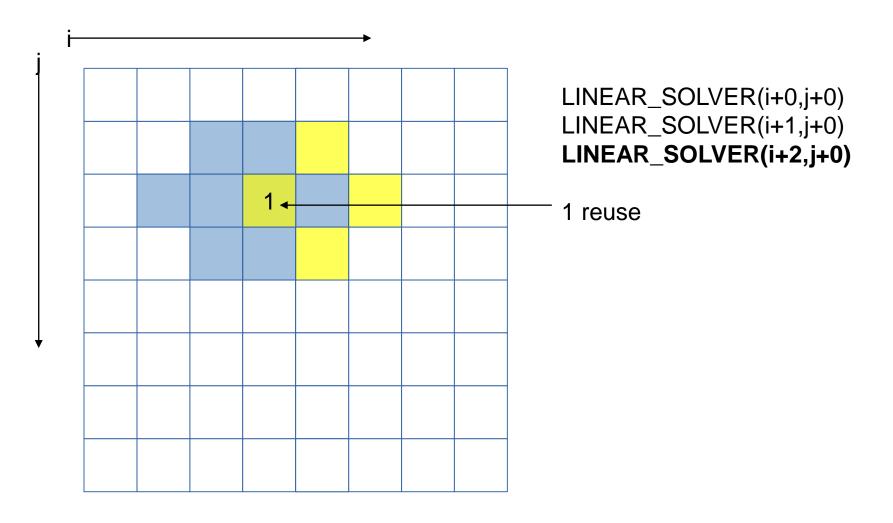
LINEAR\_SOLVER(i+0,j+0)



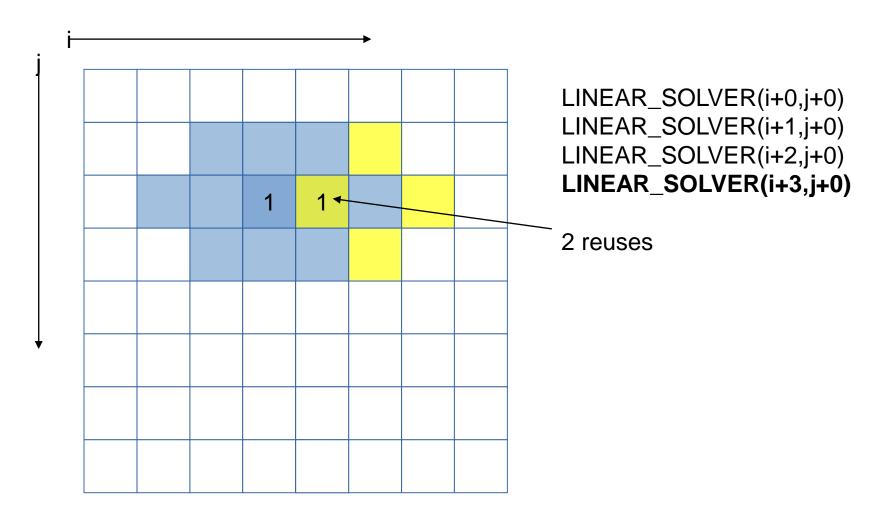


LINEAR\_SOLVER(i+0,j+0)
LINEAR\_SOLVER(i+1,j+0)

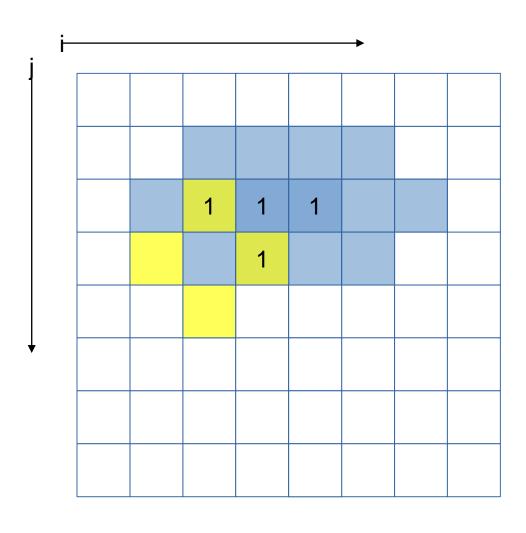












LINEAR\_SOLVER(i+0,j+0)

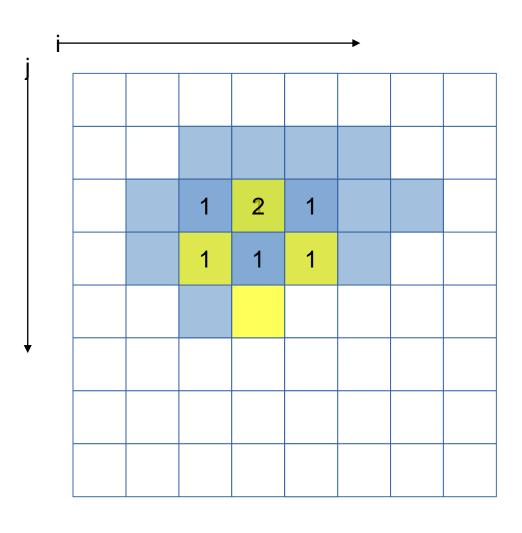
LINEAR\_SOLVER(i+1,j+0)

LINEAR\_SOLVER(i+2,j+0)

LINEAR\_SOLVER(i+3,j+0)

LINEAR\_SOLVER(i+0,j+1)





LINEAR\_SOLVER(i+0,j+0)

LINEAR\_SOLVER(i+1,j+0)

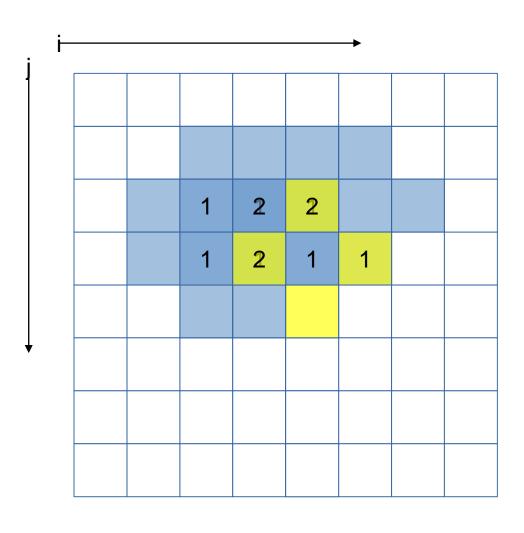
LINEAR\_SOLVER(i+2,j+0)

LINEAR\_SOLVER(i+3,j+0)

LINEAR\_SOLVER(i+0,j+1)

LINEAR\_SOLVER(i+1,j+1)





LINEAR\_SOLVER(i+0,j+0)

LINEAR\_SOLVER(i+1,j+0)

LINEAR\_SOLVER(i+2,j+0)

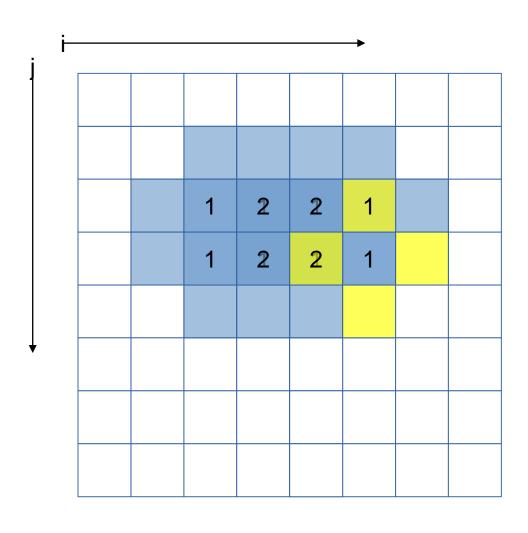
LINEAR\_SOLVER(i+3,j+0)

LINEAR\_SOLVER(i+0,j+1)

LINEAR\_SOLVER(i+1,j+1)

LINEAR\_SOLVER(i+2,j+1)



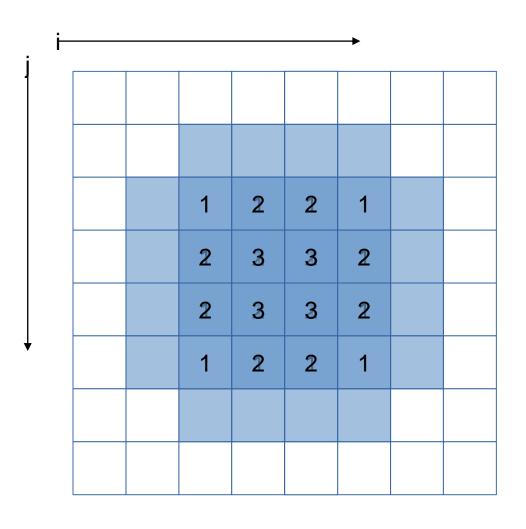


LINEAR\_SOLVER(i+0,j+0) LINEAR\_SOLVER(i+1,j+0) LINEAR\_SOLVER(i+2,j+0)

LINEAR\_SOLVER(i+3,j+0)

LINEAR\_SOLVER(i+0,j+1) LINEAR\_SOLVER(i+1,j+1) LINEAR\_SOLVER(i+2,j+1) LINEAR\_SOLVER(i+3,j+1)





LINEAR\_SOLVER(i+0-3,j+0)

LINEAR\_SOLVER(i+0-3,j+1)

LINEAR\_SOLVER(i+0-3,j+2)

LINEAR\_SOLVER(i+0-3,j+3)

# **Impacts of memory reuse**

- For the x array, instead of 4x4x4 = 64 loads, now only 32 (32 loads avoided by reuse)
- For the x0 array no reuse possible: 16 loads
- Total loads: 48 instead of 80

### 4x4 unroll

```
#define LINEARSOLVER(...) x[build index(i, j, grid size)] = ...
void linearSolver2 (...) {
  (\ldots)
 for (k=0; k<20; k++)
    for (i=1; i<=grid size-3; i+=4)
      for (j=1; j \le qrid size-3; j+=4) {
        LINEARSOLVER (..., i+0, j+0);
        LINEARSOLVER (..., i+0, j+1);
        LINEARSOLVER (..., i+0, j+2);
        LINEARSOLVER (..., i+0, j+3);
        LINEARSOLVER (..., i+1, j+0);
        LINEARSOLVER (..., i+1, j+1);
        LINEARSOLVER (..., i+1, j+2);
        LINEARSOLVER (..., i+1, j+3);
        LINEARSOLVER (..., i+2, j+0);
        LINEARSOLVER (..., i+2, j+1);
        LINEARSOLVER (..., i+2, j+2);
        LINEARSOLVER (..., i+2, j+3);
        LINEARSOLVER (..., i+3, j+0);
        LINEARSOLVER (..., i+3, j+1);
        LINEARSOLVER (..., i+3, j+2);
        LINEARSOLVER (..., i+3, j+3);
```

grid\_size must now be multiple of 4. Or loop control must be adapted (much less readable) to handle leftover iterations



### Kernel2

```
> make clean
> make KERNEL=2
> ./hydro 250 10
Cycles per element for solvers: 735.97
> magao lprof xp=sx3 -- ./hydro 250 50
> magao lprof xp=sx3 -d1 | head
Loop ID
           Function Name
                           Source Info
                                                  Time (%)
                                         Level
143
          linearSolver2
                         14,167@kernel.c
                                        Innermost
                                                  57.14
          c densitySolver | 14,167@kernel.c
 55
                                        Innermost
                                                  19.64
 76
          c velocitySolver |
                         14,283@kernel.c
                                        Innermost
                                                  3.57
> magao cga hydro loop=143
```

Remark: less calls were unrolled since linearSolver is now much more bigger

### **CQA output for kernel2**

```
Matching between your loop ...
                                           4x4 Unrolling were applied
The binary loop is composed of 96 FP
arithmetical operations:
 - 64: addition or subtraction
 - 32: multiply
The binary loop is loading 272 bytes
                                         → Expected 48... But still better
(68 single precision FP elements). -
The binary loop is storing 64 bytes
                                           than 80
(16 single precision FP elements).
```



### **Summary of optimizations and gains**

