MAQAO
Hands-on exercises

Profiling bt-mz (incl. scalability)
Optimising a code

Setup (reminder)

Login to the cluster

```
> ssh <username>@lxlogin10.lrz.de
```

Copy handson material to your workspace directory

```
> export TW40=/lrz/sys/courses/vihps
> export WORK=$SCRATCH # assumed fastest filesystem
Hint: copy in ~/.bash_profile
> cd $WORK
> tar xvf $TW40/material/maqao/MAQAO_HANDSON.tgz
> tar xvf $TW40/material/maqao/NPB3.4-MZ-MPI.tgz
```

Load MAQAO environment

```
> module use $TW40/modulefiles
> module load maqao
```

Setup (bt-mz compilation with Intel compiler and MPI & debug symbols)

Go to the NPB directory provided with MAQAO handsons

```
> cd $WORK/NPB3.4-MZ-MPI
```

Load Intel compiler and environment (if not already loaded)

```
> module load devEnv/Intel/2019
```

Compile and run

```
> make bt-mz CLASS=C
> cd bin
> cp $WORK/MAQAO_HANDSON/bt/bt.sbatch .
> sbatch bt.sbatch
```

Remark: with version 3.4 the generated executable supports any number of ranks (no need to generate one executable for 6 ranks, another for 8 etc.)

Profiling bt-mz with MAQAO

Salah Ibnamar

Setup ONE View for batch mode

The ONE View configuration file must contain all variables for executing the application.

Retrieve the configuration file prepared for bt-mz in batch mode from the MAQAO_HANDSON directory

```
> cd $WORK/NPB3.4-MZ-MPI/bin
> cp $WORK/MAQAO_HANDSON/bt/bt_OV_sbatch.lua .
> less bt_OV_sbatch.lua
```

```
binary = "bt-mz.C.x"
...
batch_script = "bt_maqao.sbatch"
batch_command = "sbatch <batch_script>"
...
number_processes = 4
number_processes_per_node = 2
omp_num_threads = 8
...
mpi_command = "mpirun -n <number_processes>"
...
```

Review jobscript for use with ONE View

All variables in the jobscript defined in the configuration file must be replaced with their name from it.
Retrieve jobscript modified for ONE View from the MAQAO_HANDSON directory.

```
> cd $WORK/NPB3.4-MZ-MPI/bin #if current directory has changed
> cp $WORK/MAQAO_HANDSON/bt/bt_maqao.sbatch .
> less bt_maqao.sbatch
```

```
...
#SBATCH --ntasks-per-node=2<number_processes_per_node>
#SBATCH --cpus-per-task=8<omp_num_threads>
...
export OMP_NUM_THREADS=8<omp_num_threads>
...
mpirun -n ... $EXE
<mpi_command> <run_command>
...
```

Launch MAQAO ONE View on bt-mz (batch mode)

Launch ONE View

```
> cd $WORK/NPB3.4-MZ-MPI/bin #if current directory has changed
> maqao oneview -R1 --config=bt_OV_sbatch.lua -xp=ov_sbatch
```

The -xp parameter allows to set the path to the experiment directory, where ONE View stores the analysis results and where the reports will be generated.
If -xp is omitted, the experiment directory will be named maqao_<timestamp>.

WARNINGS:

- If the directory specified with -xp already exists, ONE View will reuse its content but not overwrite it.

(OPTIONAL) Setup ONE View for interactive mode

Retrieve the configuration file prepared for bt-mz in interactive mode from the MAQAO_HANDSON directory

```
> cd $WORK/NPB3.4-MZ-MPI/bin #if current directory has changed
> cp $WORK/MAQAO_HANDSON/bt/bt_OV_interact.lua .
> less bt_OV_interact.lua
```

```
binary = "bt-mz.C.x"
...
number_processes = 4
number_processes_per_node = 2
...
omp_num_threads = 8
...
mpi_command = "mpirun -n <number_processes>"
```

(OPTIONAL) Launch MAQAO ONE View on bt-mz (interactive mode)

Request interactive session with 2 nodes

```
> srun -M ivymuc --reservation=hhps1s21_workshop \
--nodes=2 --pty bash
```

Launch ONE View

```
> cd $WORK/NPB3.4-MZ-MPI/bin
> maqao oneview -R1 --config=bt_OV_interact.lua \
-xp=ov_interactive
```

Exit interactive session

```
> exit
```

Display MAQAO ONE View results

The HTML files are located in **<exp-dir>/RESULTS/<binary>_one_html**, where *<exp-dir>* is the path of he experiment directory (set with -xp) and *<binary>* the name of the executable.

Mount $WORK locally:

```
> mkdir ivymuc_work
> sshfs <user>@lxlogin10.lrz.de:/gpfs/scratch/a2c06/<user> \
ivymuc_work
> firefox ivymuc_work/NPB3.4-MZ-MPI/bin/ov_sbatch/RESULTS/bt-
mz.C.x_one_html/index.html
```

It is also possible to compress and download the results to display them:

```
> tar czf $HOME/bt_html.tgz ov_sbatch/RESULTS/bt-mz.C.x_one_html
```

```
> scp <user>@lxlogin10.lrz.de:bt_html.tgz .
> tar xf bt_html.tgz
> firefox ov_sbatch/RESULTS/bt-mz.C.x_one_html/index.html
```

sshfs & scp hints

- To install sshfs on Debian-based Linux distributions (like Ubuntu)

```
> sudo apt install sshfs
```

- Recommended to close a sshfs directory after use

```
> fusermount -u /path/to/sshfs/directory
```

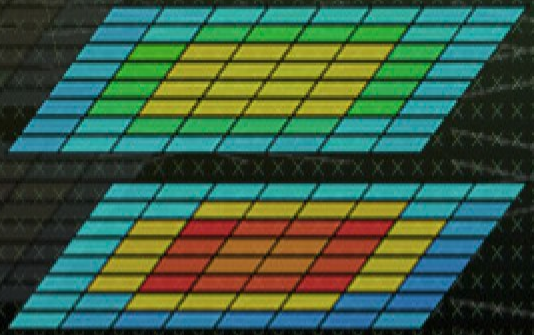
- scp is slow to copy directories (especially when containing many small files), copy a .tgz archive of the directory

Display MAQAO ONE View results (optional)

A sample result directory is in **`MAQAO_HANDSON/bt/bt_html_example.tgz`**

Results can also be viewed directly on the console in text mode:

```
> maqao oneview -R1 -xp=ov_sbatch --output-format=text
```



Scalability profiling of bt-mz with MAQAO

Salah Ibnamar

Setup ONE View for scalability analysis

Retrieve the configuration file prepared for bt-mz in batch mode from the MAQAO_HANDSON directory

```
> cd $WORK/NPB3.4-MZ-MPI/bin #if cur. dir. has changed
> cp $WORK/MAQAO_HANDSON/bt/bt_OV_scal.lua .
> less bt_OV_scal.lua
```

```
binary = "./bt-mz.C.x"
...
run_command = "<binary>"
...
batch_script = "bt_maqao.sbatch"
...
batch_command = "sbatch <batch_script>"
...
number_processes = 4
...
number_processes_per_node = 4
...
omp_num_threads = 1
...
mpi_command = "mpirun -n <number_processes>"
...
multiruns_params = {
 {number_processes = 1, omp_num_threads = 8, number_processes_per_node = 1},
 {number_processes = 4, omp_num_threads = 1, number_processes_per_node = 2},
 {number_processes = 4, omp_num_threads = 8, number_processes_per_node = 2},
}
scalability_reference = "lowest-threads"
```

Launch MAQAO ONE View on bt-mz (scalability mode)

Launch ONE View (execution will be longer!)

```
> maqao oneview -R1 --with-scalability=on \
-c=bt_OV_scal.lua -xp=ov_scal
```

The results can then be accessed similarly to the analysis report.

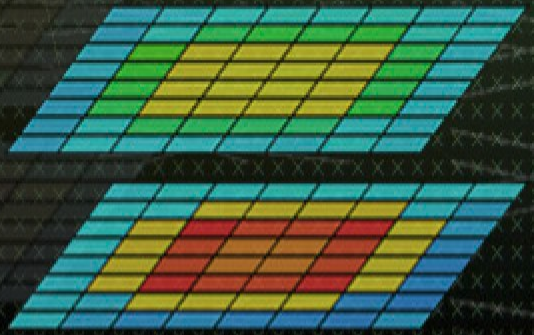
```
> firefox ivymuc_work/NPB3.4-MZ-MPI/bin/ov_scal/RESULTS/bt-
mz.C.x_one_html/index.html
```

OR

```
> tar czf $HOME/bt_scal.tgz \
ov_scal/RESULTS/bt-mz.C.x_one_html
```

```
> scp <user>@lxlogin10.lrz.de:ov_scal.tgz .
> tar xf ov_scal.tgz
> firefox ov_scal/RESULTS/bt-mz.C.x_one_html/index.html
```

A sample result directory is in **MAQAO_HANDSON/bt/bt_scal_html_example.tgz**



Optimising a code with MAQAO

Emmanuel OSERET

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

Compile with GNU compiler

Go to the handson directory

```
> cd $WORK/MAQAO_HANDSON/matmul
```

Compile all variants (must be done on login node)

```
> module load gcc/9
> make all
```

Load MAQAO environment

```
> module use $TW40/modulefiles
> module load maqao
```

Setup matmul for srun-direct run from Oneview

The ONE View configuration file must contain all variables for executing the application.

```
> cd $WORK/MAQAO_HANDSON/matmul #if cur. directory has changed
> less ov_orig.lua
```

```
binary = "matmul_orig"
run_command = "<binary> 400 300" -- <size of matrix> <number of repetitions>
...
number_processes_per_node = 1
mpi_command = "srun -M ivymuc --reservation=hhps1s21_workshop --exclusive"
...
```

Analysing matrix multiply with MAQAO

Analyse matrix multiply with ONE View

```
> maqao oneview -R1 -c=ov_orig.lua -xp=ov_orig
```

Viewing results (HTML)

On your local machine (sshfs):

```
> firefox ivymuc_work/MAQAO_HANDSON/matmul/ov_orig/RESULTS/
matmul_orig_one_html/index.html &
```

Global Metrics

Total Time (s)		26.16
Profiled Time (s)		26.16
Time in loops (%)		100
Time in innermost loops (%)		99.87
Time in user code (%)		100
Compilation Options		**matmul_orig**: -march=(target) is missing. -funroll-loops is missing.
Perfect Flow Complexity		1.00
Array Access Efficiency (%)		83.32
Perfect OpenMP + MPI + Pthread		1.00
Perfect OpenMP + MPI + Pthread + Perfect Load Distribution		1.00
No Scalar Integer	Potential Speedup	1.00
	Nb Loops to get 80%	1
FP Vectorised	Potential Speedup	2.00
	Nb Loops to get 80%	1
Fully Vectorised	Potential Speedup	7.99
	Nb Loops to get 80%	1
FP Arithmetic Only	Potential Speedup	1.00
	Nb Loops to get 80%	1

CQA output for the baseline kernel

Vectorization

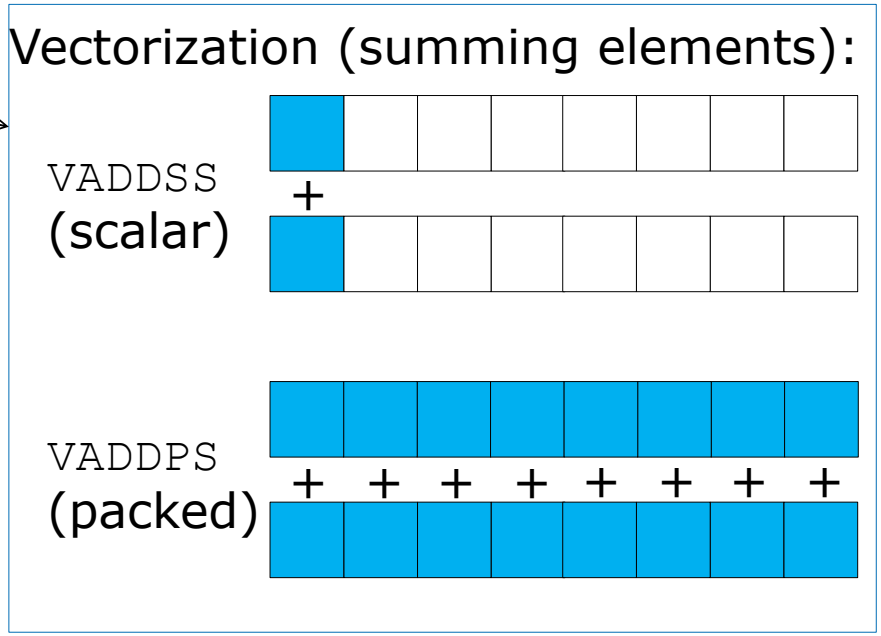
Your loop is not vectorized. 8 data elements could be processed at once in vector registers. By vectorizing your loop, you can lower the cost of an iteration from 3.00 to 0.37 cycles (8.00x speedup).

Details

All SSE/AVX instructions are used in scalar version (process only one data element in vector registers). Since your execution units are vector units, only a vectorized loop can use their full power.

Workaround

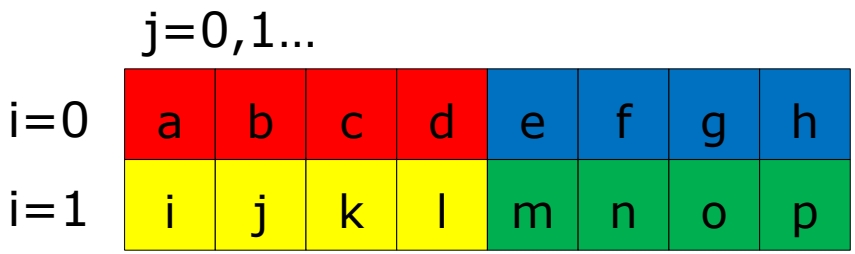
- Try another compiler or update/tune your current one:
  - recompile with fassociative-math (included in Ofast or ffast-math) to extend loop vectorization to FP reductions.
- Remove inter-iterations dependences from your loop and make it unit-stride:
  - If your arrays have 2 or more dimensions, check whether elements are accessed contiguously and, otherwise, try to permute loops accordingly: C storage order is row-major: for(i) for(j) a[j][i] = b[j][i]; (slow, non stride 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 structures of arrays instead (SoA): for(i) a[i].x = b[i].x; (slow, non stride 1) => for(i) a.x[i] = b.x[i]; (fast, stride 1)



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

Impact of loop permutation on data access

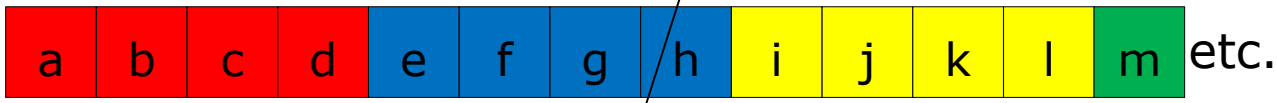
Logical mapping



Efficient vectorization + prefetching

Physical mapping

(C stor. order: row-major)




```
for (j=0; j<n; j++)
  for (i=0; i<n; i++)
    f(a[i][j]);
```


```
for (i=0; i<n; i++)
  for (j=0; j<n; j++)
    f(a[i][j]);
```

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

```
void kernel1 (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];
  }
}
```

Analyse matrix multiply with permuted loops

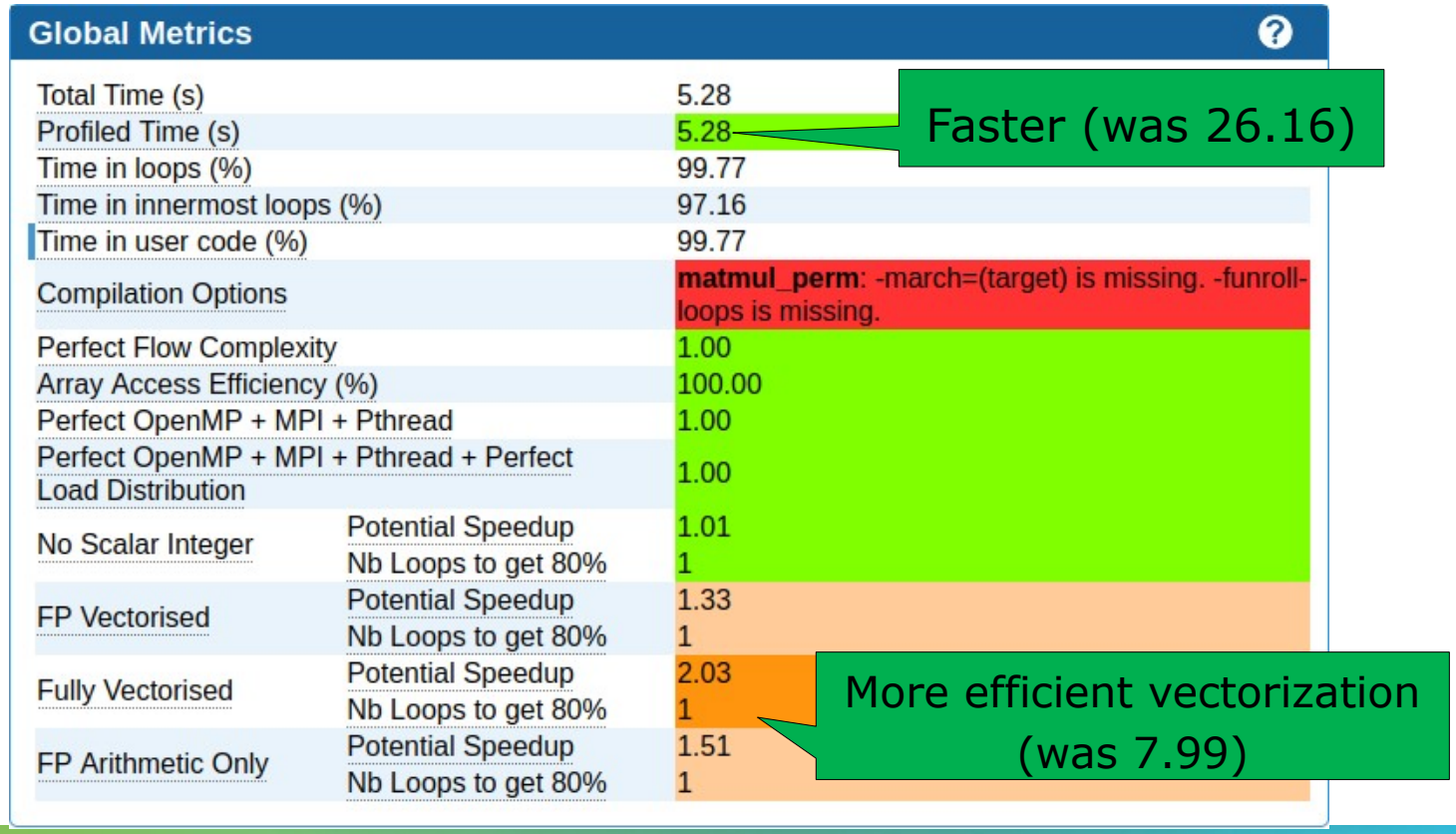
Analyse matrix multiply with ONE View

```
> maqao oneview -R1 -c=ov_perm.lua -xp=ov_perm
```

Viewing results (HTML)

On your local machine (sshfs):

```
> firefox ivymuc_work/MAQAO_HANDSON/matmul/ov_perm/RESULTS/
matmul_perm_one_html/index.html &
```



Global Metrics

Total Time (s)		5.28
Profiled Time (s)		5.28
Time in loops (%)		99.77
Time in innermost loops (%)		97.16
Time in user code (%)		99.77
Compilation Options		**matmul_perm**: -march=(target) is missing. -funroll-loops is missing.
Perfect Flow Complexity		1.00
Array Access Efficiency (%)		100.00
Perfect OpenMP + MPI + Pthread		1.00
Perfect OpenMP + MPI + Pthread + Perfect Load Distribution		1.00
No Scalar Integer	Potential Speedup	1.01
	Nb Loops to get 80%	1
FP Vectorised	Potential Speedup	1.33
	Nb Loops to get 80%	1
Fully Vectorised	Potential Speedup	2.03
	Nb Loops to get 80%	1
FP Arithmetic Only	Potential Speedup	1.51
	Nb Loops to get 80%	1

CQA output after loop permutation

gain | potential | hint | expert

Vectorization

Your loop is vectorized, but using only 128 out of 256 bits (SSE/AVX-128 instructions on AVX/AVX2 processors). By fully vectorizing your loop, you can lower the cost of an iteration from 2.00 to 1.00 cycles (2.00x speedup).

Details

All SSE/AVX instructions are used in vector version (process two or more data elements in vector registers). Since your execution units are vector units, only a fully vectorized loop can use their full power.

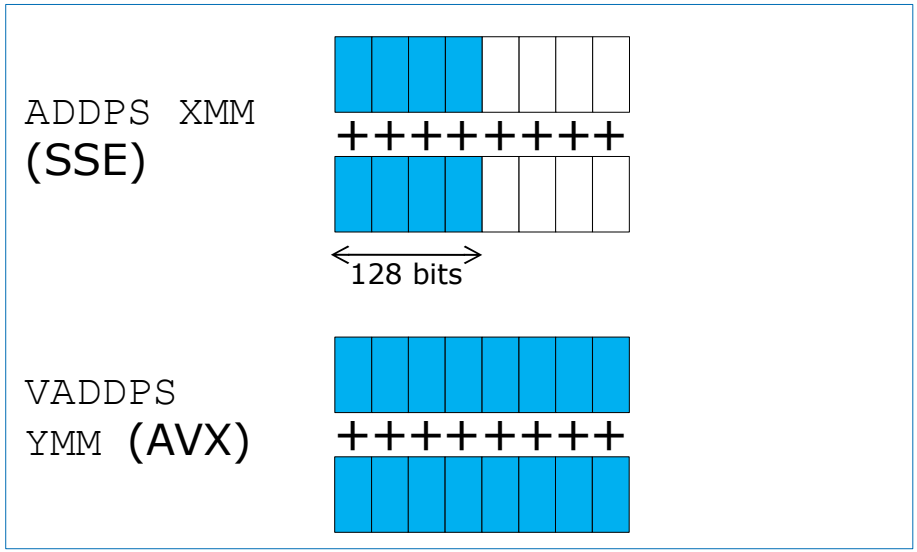
Workaround

- Recompile with march=core-avx-i. CQA target is Core_i7X_Xeon_E5E7_v2 (Intel Xeon processor E5-2
  Xeon processor E5-2400 v2 and E7-8800/4800/2800 v2 product families based on Ivy Bridge-E microarchitecture, Intel Core i7-49xx Processor Extreme Edition) but specialization flags are -march=x86-64
- Use vector aligned instructions:
  1. align your arrays on 32 bytes boundaries: replace { void *p = malloc (size); } with { void *p; posix_memalign (&p, 32, size); }.
  2. inform your compiler that your arrays are vector aligned: if array 'foo' is 32 bytes-aligned, define a pointer 'p_foo' as __builtin_assume_aligned (foo, 32) and use it instead of 'foo' in the loop.

Let’s try this

Impacts of architecture specialization: vectorization

- Vectorization
  - SSE instructions (SIMD 128 bits) used on a processor supporting AVX256 ones (SIMD 256 bits)
  - => 50% efficiency loss



Analyse matrix multiply with microarchitecture-specialization and array alignment (requires size%8=0)

Analyse matrix multiply with ONE View

```
> maqao oneview -R1 -c=ov_align.lua -xp=ov_align
```

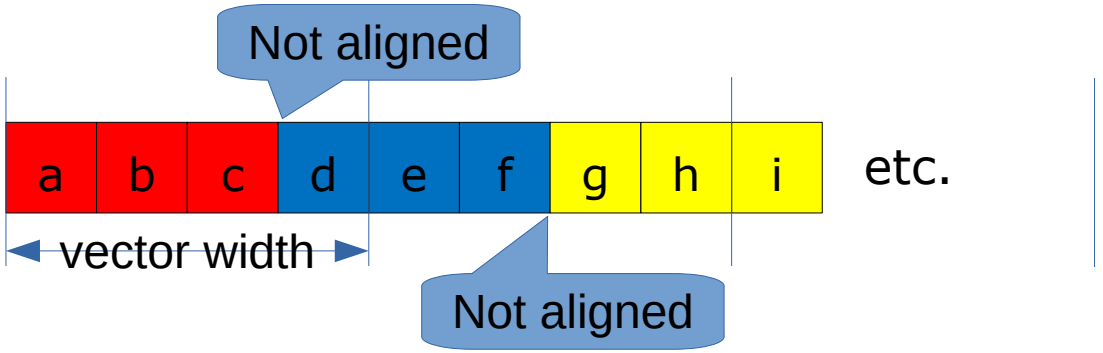
Checkout program output (in lprof.log)

```
> cat ov_align/logs/lprof.log
driver.c: Using posix_memalign instead of malloc
```

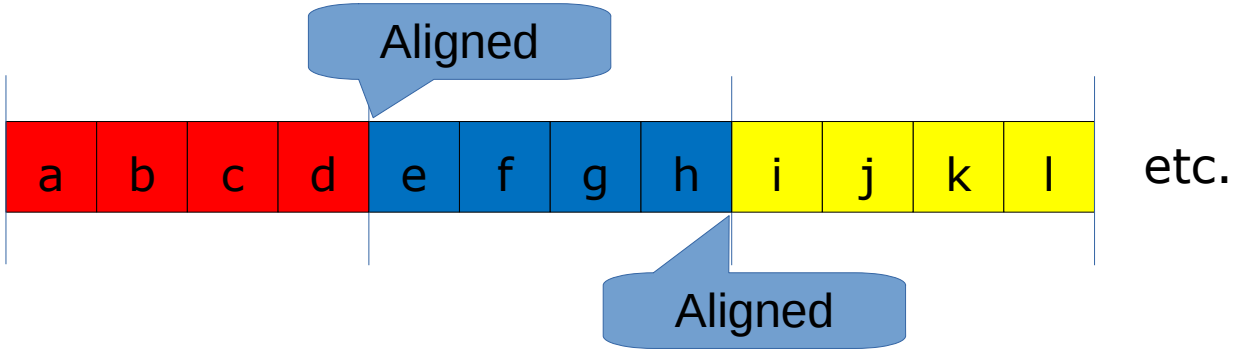
Multidimensional array alignment

Data organized as a 2D array: n lines of 3 columns
Each vector can hold 4 consecutive elements

a[n][3], only 1st element is aligned



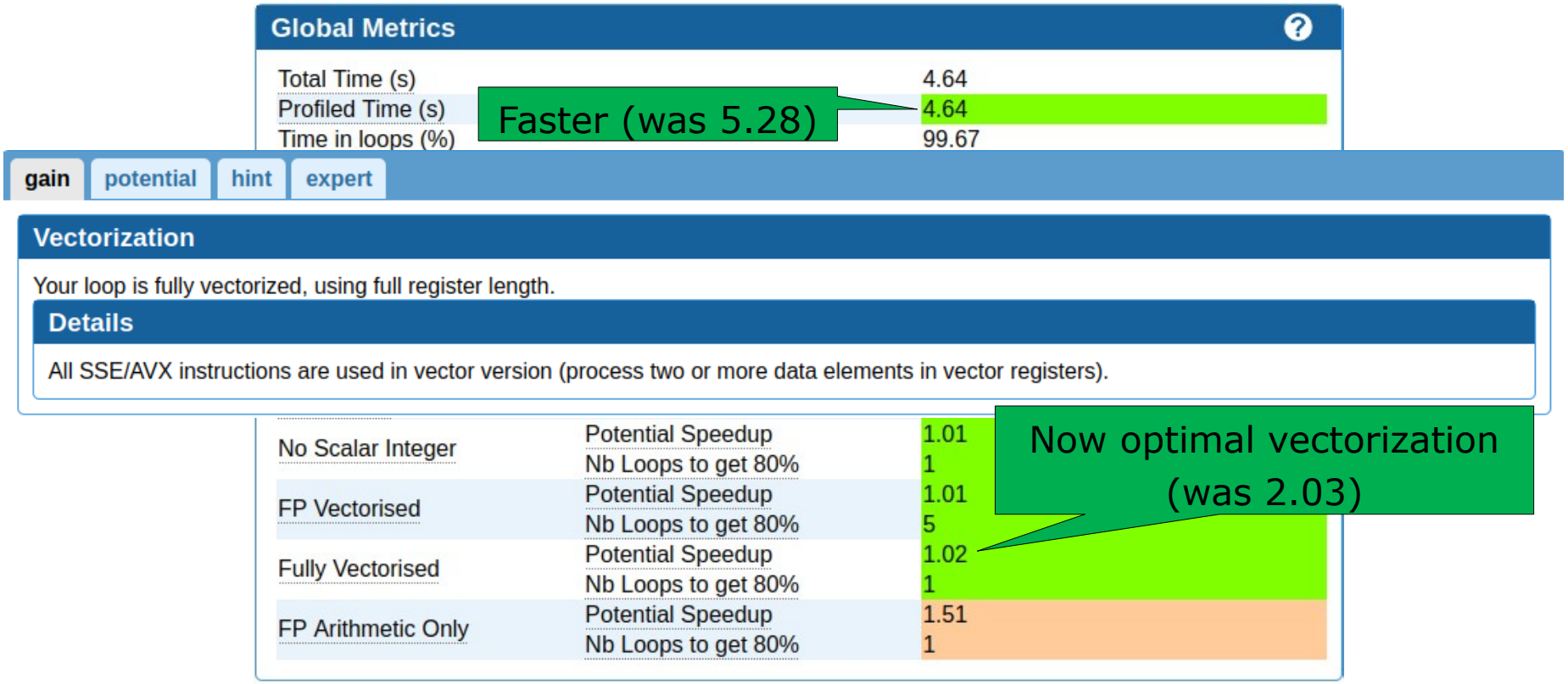
a[n][4], 1st element of each line are aligned



Viewing results (HTML)

On your local machine (sshfs):

```
> firefox ivymuc_work/MAQAO_HANDSON/matmul/ov_align/RESULTS/
matmul_align_one_html/index.html &
```



Viewing results (HTML)

Global Metrics

Total Time (s)		4.64
Profiled Time (s)		4.64
Time in loops (%)		99.67
Time in innermost loops (%)		96.83
Time in user code (%)		99.68
Compilation Options		**matmul_align**: -funroll-loops is missing.
Perfect Flow Complexity		1.00
Array Access Efficiency (%)		100.00
Perfect OpenMP + MPI + Pthread		1.00
Perfect OpenMP + MPI + Pthread + Perfect Load Distribution		1.00
No Scalar Integer	Potential Speedup	1.01
	Nb Loops to get 80%	1
FP Vectorised	Potential Speedup	1.01
	Nb Loops to get 80%	5
Fully Vectorised	Potential Speedup	1.02
	Nb Loops to get 80%	1
FP Arithmetic Only	Potential Speedup	1.51
	Nb Loops to get 80%	1

Let's try this

Analyse matrix multiply with loop unrolling

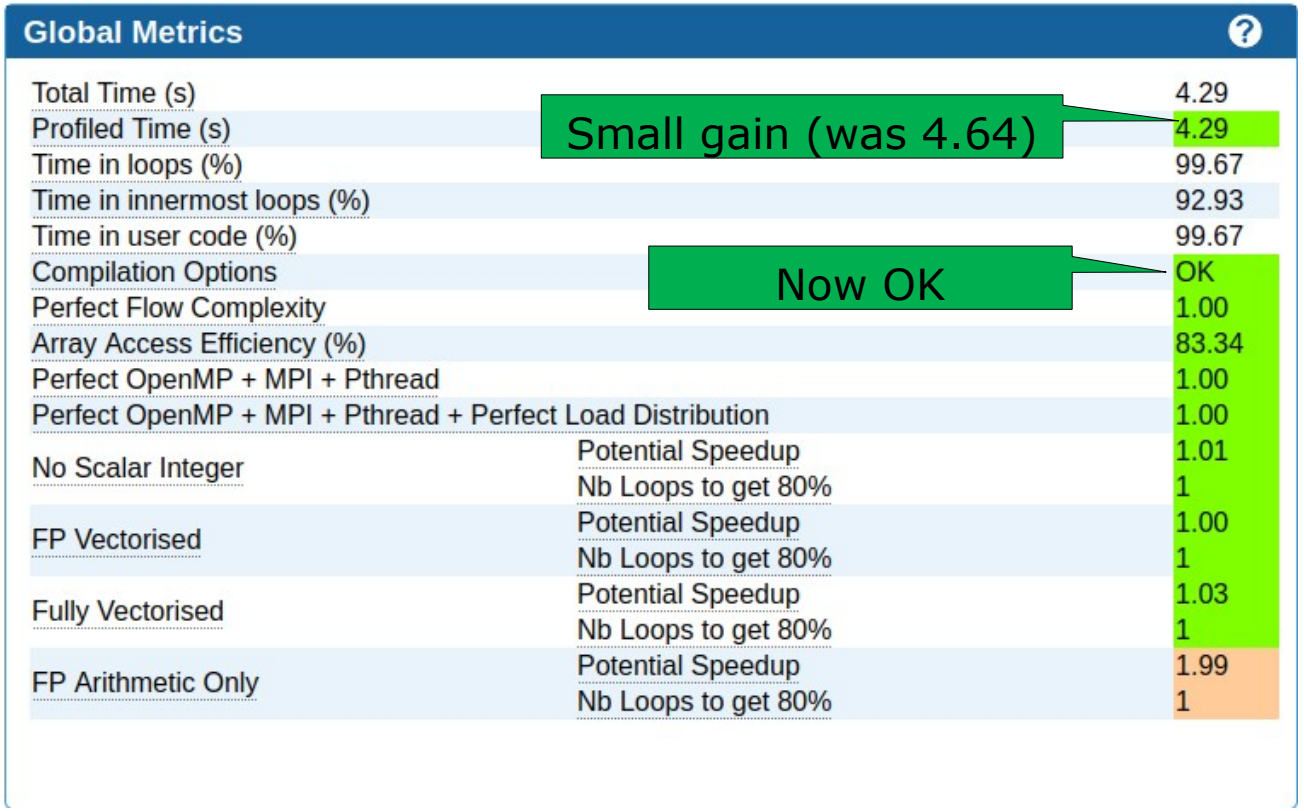
Analyse matrix multiply with ONE View

```
> maqao oneview -R1 -c=ov_unroll.lua -xp=ov_unroll
```

Viewing results (HTML)

On your local machine (sshfs):

```
> firefox ivymuc_work/MAQAO_HANDSON/matmul/ov_unroll/RESULTS/
matmul_unroll_one_html/index.html &
```



Total Time (s)		4.29
Profiled Time (s)		4.29
Time in loops (%)		99.67
Time in innermost loops (%)		92.93
Time in user code (%)		99.67
Compilation Options		OK
Perfect Flow Complexity		1.00
Array Access Efficiency (%)		83.34
Perfect OpenMP + MPI + Pthread		1.00
Perfect OpenMP + MPI + Pthread + Perfect Load Distribution		1.00
No Scalar Integer	Potential Speedup	1.01
	Nb Loops to get 80%	1
FP Vectorised	Potential Speedup	1.00
	Nb Loops to get 80%	1
Fully Vectorised	Potential Speedup	1.03
	Nb Loops to get 80%	1
FP Arithmetic Only	Potential Speedup	1.99
	Nb Loops to get 80%	1

Using comparison mode (iso-source)

```
> maqao oneview --compare-reports --inputs=ov_orig,ov_unroll \
-xp=ov_orig_vs_unroll
```

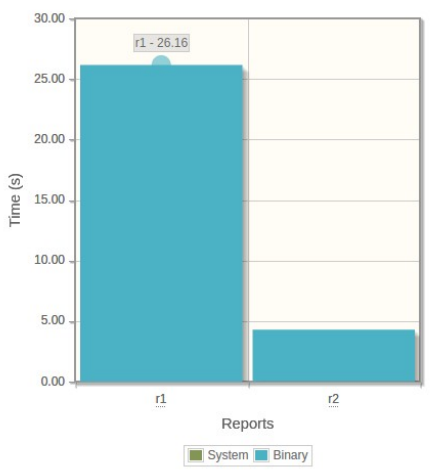
Remark: open `ov_orig_vs_unroll/index.html` (xp is directly a HTML directory)

Global Metrics

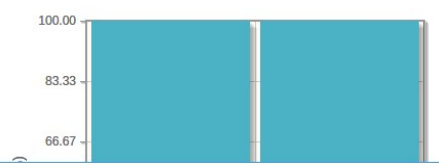
Metric		r1	r2
Total Time (s)		26.16	4.29
Profiled Time (s)		26.16	4.29
Time in loops (%)		100.00	99.67
Time in innermost loops (%)		99.87	92.93
Time in user code (%)		100	99.67
Compilation Options		**matmul_orig**: -march=(target) is missing. -funroll-loops is missing.	OK
Perfect Flow Complexity		1.00	1.00
Array Access Efficiency (%)		83.32	83.34
Perfect OpenMP + MPI + Pthread		1.00	1.00
Perfect OpenMP + MPI + Pthread + Perfect Load Distribution		1.00	1.00
No Scalar Integer	Potential Speedup	1.00	1.01
	Nb Loops to get 80%	1	1
FP Vectorised	Potential Speedup	2.00	1.00
	Nb Loops to get 80%	1	1
Fully Vectorised	Potential Speedup	7.99	1.03
	Nb Loops to get 80%	1	1
Only FP Arithmetic	Potential Speedup	1.00	1.99
	Nb Loops to get 80%	1	1

Application Categorization

Time



Coverage



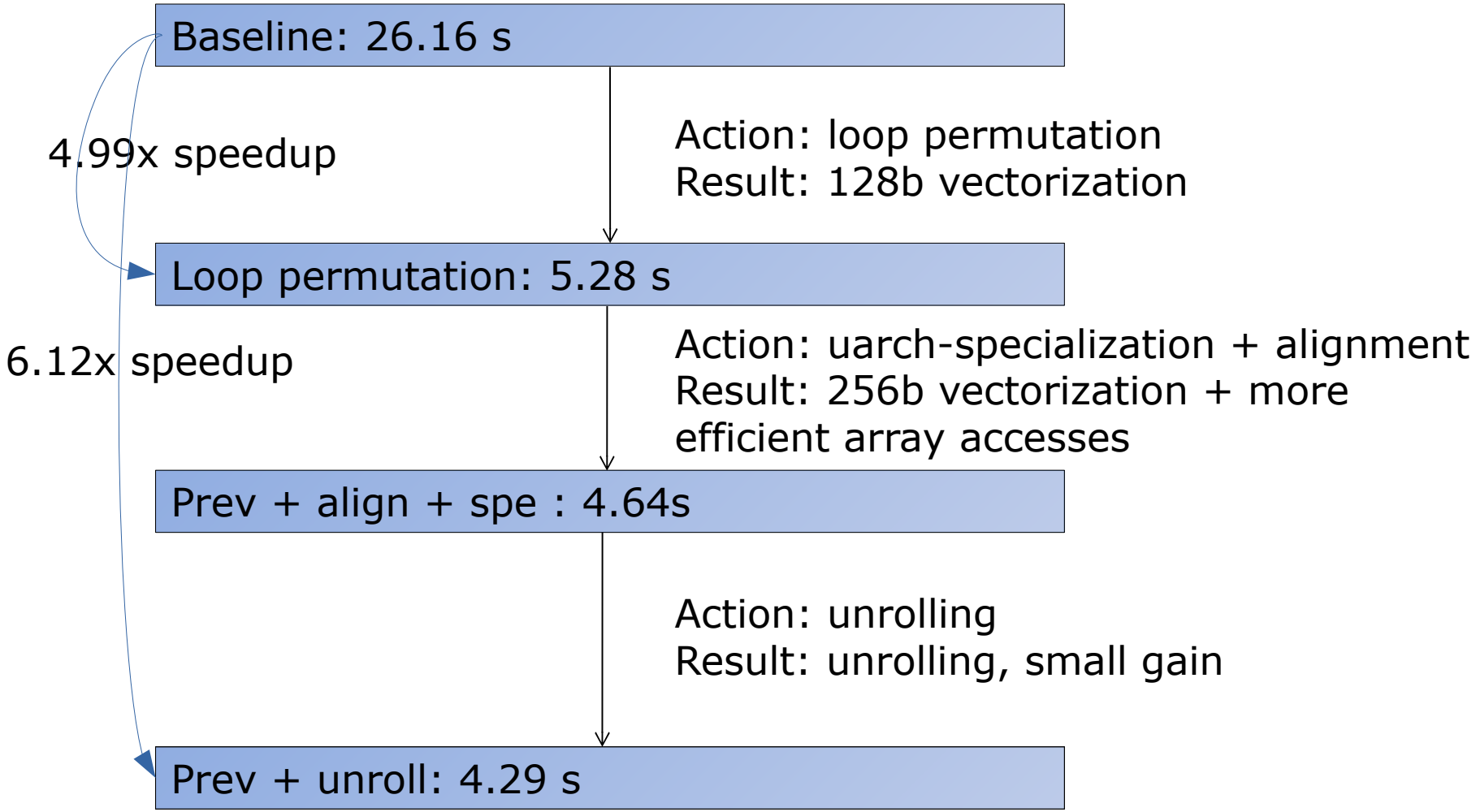
Experiment Summaries

	r1	r2
Application	./matmul_orig	./matmul_unroll
Timestamp		
Experiment Type	Sequential	Sequential
Machine	ivynsr0r1is07	ivynsr0r1is07
Architecture	x86_64	x86_64
Micro Architecture	IVY_BRIDGE_E	IVY_BRIDGE_E
Model Name	Intel(R) Xeon(R) CPU E5-2650 v2 @ 2.60GHz	Intel(R) Xeon(R) CPU E5-2650 v2 @ 2.60GHz
Cache Size	20480 KB	20480 KB
Number of Cores	8	8
Maximal Frequency	3.4 GHz	3.4 GHz
OS Version	Linux 4.4.180-94.100-default #1 SMP Tue Jul 9 19:57:20 UTC 2019 (1569ffb)	Linux 4.4.180-94.100-default #1 SMP Tue Jul 9 19:57:20 UTC 2019 (1569ffb)
Architecture used during static analysis	x86_64	x86_64
Micro Architecture used during static analysis	IVY_BRIDGE_E	IVY_BRIDGE_E
Compilation Options	**matmul_orig**: GNU 9.2.0 -mtune=generic -march=x86-64 -g -O3 -fno-omit-frame-pointer	**matmul_unroll**: GNU 9.2.0 -march=ivybridge -g -O3 -funroll-loops -fno-omit-frame-pointer
Number of processes observed	1	1
Number of threads observed	1	1
MAQAO version	2.13.10	2.13.10
MAQAO build	357719356ff88ecffcd8d699db3b2bc4524d3c25::20210604-185701	357719356ff88ecffcd8d699db3b2bc4524d3c25::20210604-185701

Functions

Name	Module	Coverage (%)		Time (s)		Nb Threads		Deviation (coverage)	
		run 1	run 2	run 1	run 2	run 1	run 2	run 1	run 2
kernel	binary	100	99.65	26.16	4.27	1	1	0.00	0.00
__GI_memset	libc-2.22.so	0	0.26		0.01		1		0.00
__random_r	libc-2.22.so	0	0.02		0		1		0.00
rand	libc-2.22.so	0	0.02		0		1		0.00
__random	libc-2.22.so	0	0.02		0		1		0.00
init_mat	binary	0	0.02		0		1		0.00

Summary of optimizations and gains



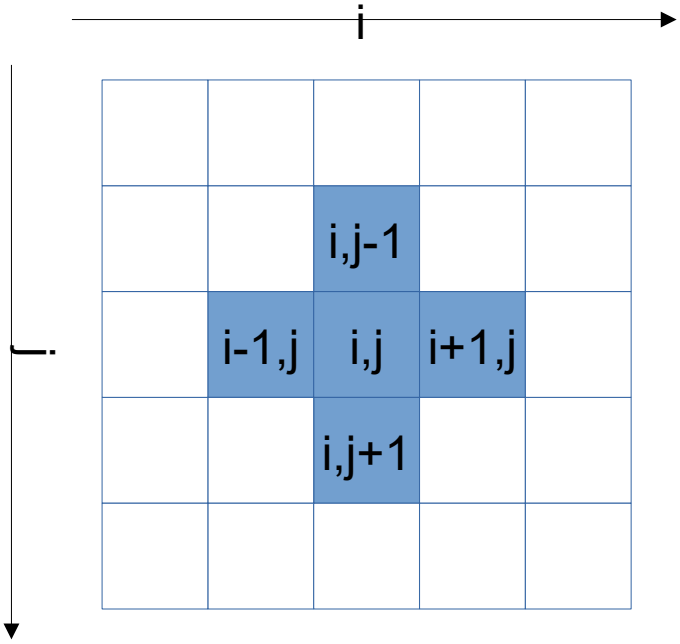
Hydro code

```
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++)
        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



Compile with Intel compiler on login node

Switch to the hydro handson folder

```
> cd $WORK/MAQAO_HANDSON/hydro
```

Load MAQAO (if no more loaded)

```
> module use $TW40/modulefiles
> module load maqao
```

Load Intel 19 compiler (if no more loaded)

```
> module load devEnv/Intel/2019
```

Compile

```
> make
```

Setup hydro for srun-direct run from Oneview

The ONE View configuration file must contain all variables for executing the application.

```
> cd $WORK/MAQAO_HANDSON/hydro #if cur. directory has changed
> less ov_k0.lua
```

```
binary = "./hydro_k0"
run_command = "<binary> 300 200" -- <size of matrix> <number of repetitions>
...
number_processes_per_node = 1
mpi_command = "srun -M ivymuc --reservation=hhps1s21_workshop --exclusive"
...
```

Running and analyzing kernel0

Profile with MAQAO

```
> maqao oneview -R1 -xp=ov_k0 -c=ov_k0.lua
```

Viewing results (HTML)

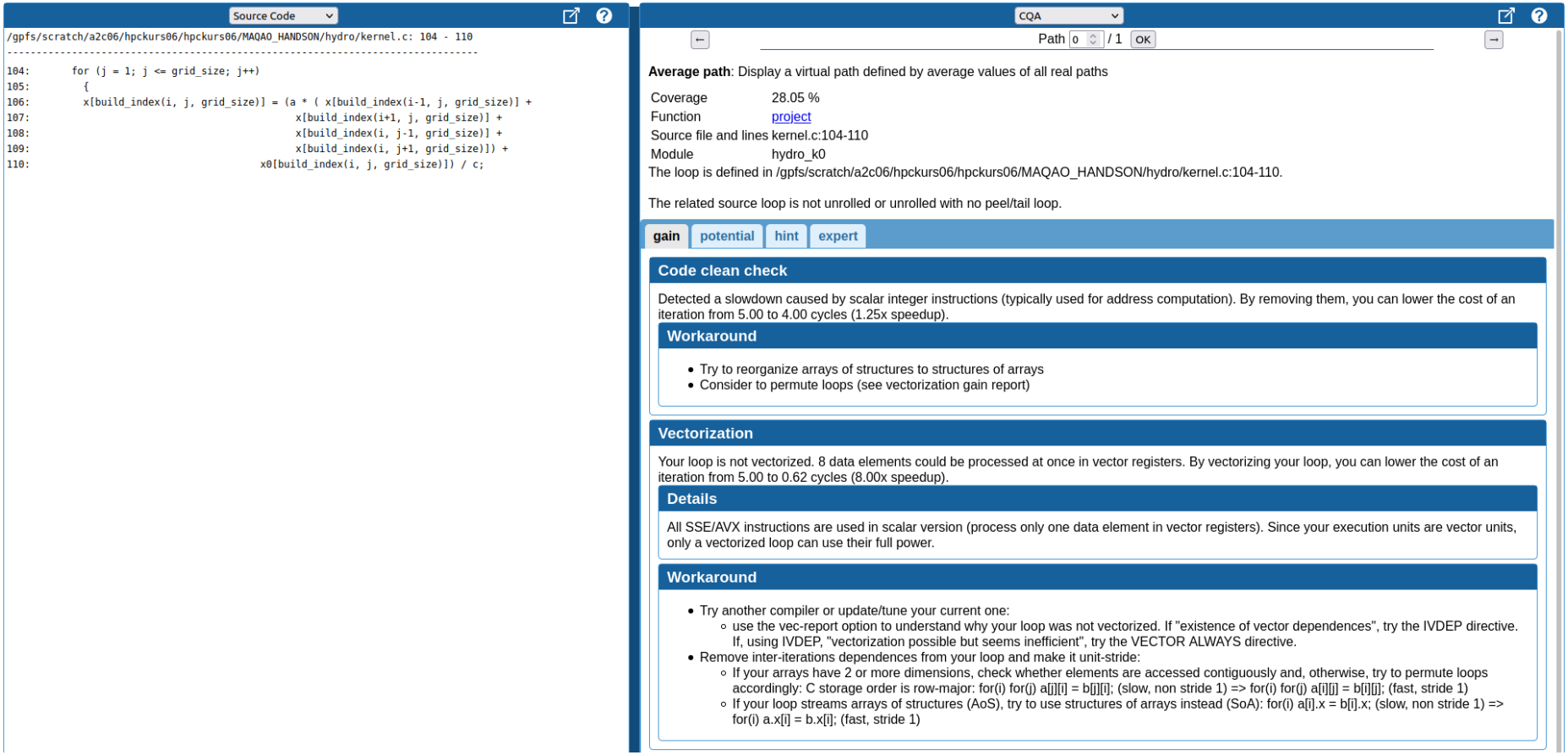
On your local machine (sshfs):

```
> firefox ivymuc_work/MAQAO_HANDSON/hydro/ov_k0/RESULTS/
hydro_k0_one_html/index.html &
```

Global Metrics

Total Time (s)		19.76
Profiled Time (s)		19.76
Time in loops (%)		100.03
Time in innermost loops (%)		99.93
Time in user code (%)		99.97
Compilation Options		OK
Perfect Flow Complexity		1.04
Array Access Efficiency (%)		50.57
Perfect OpenMP + MPI + Pthread		1.00
Perfect OpenMP + MPI + Pthread + Perfect Load Distribution		1.00
No Scalar Integer	Potential Speedup	1.06
	Nb Loops to get 80%	1
FP Vectorised	Potential Speedup	1.98
	Nb Loops to get 80%	4
Fully Vectorised	Potential Speedup	4.58
	Nb Loops to get 80%	6
FP Arithmetic Only	Potential Speedup	1.12
	Nb Loops to get 80%	5

Running and analyzing kernel0



CQA output for kernel0

The related source loop is not unrolled or unrolled with no peel/tail loop.

gain | potential | **hint** | expert

Slow data structures access

Detected data structures (typically arrays) that cannot be efficiently read/written

Details

- Constant unknown stride: 4 occurrence(s)

Non-unit stride (uncontiguous) accesses are not efficiently using data caches

Workaround

- Try to reorganize arrays of structures to structures of arrays
- Consider to permute loops (see vectorization gain report)

Type of elements and instruction set

5 SSE or AVX instructions are processing arithmetic or math operations on single precision FP elements in scalar mode (one at a time).

Matching between your loop (in the source code) and the binary loop

The binary loop is composed of 5 FP arithmetical operations:

- 4: addition or subtraction
- 1: multiply

The binary loop is loading 20 bytes (5 single precision FP elements). The binary loop is storing 4 bytes (1 single precision FP elements).

Arithmetic intensity

Arithmetic intensity is 0.21 FP operations per loaded or stored byte.

Unroll opportunity

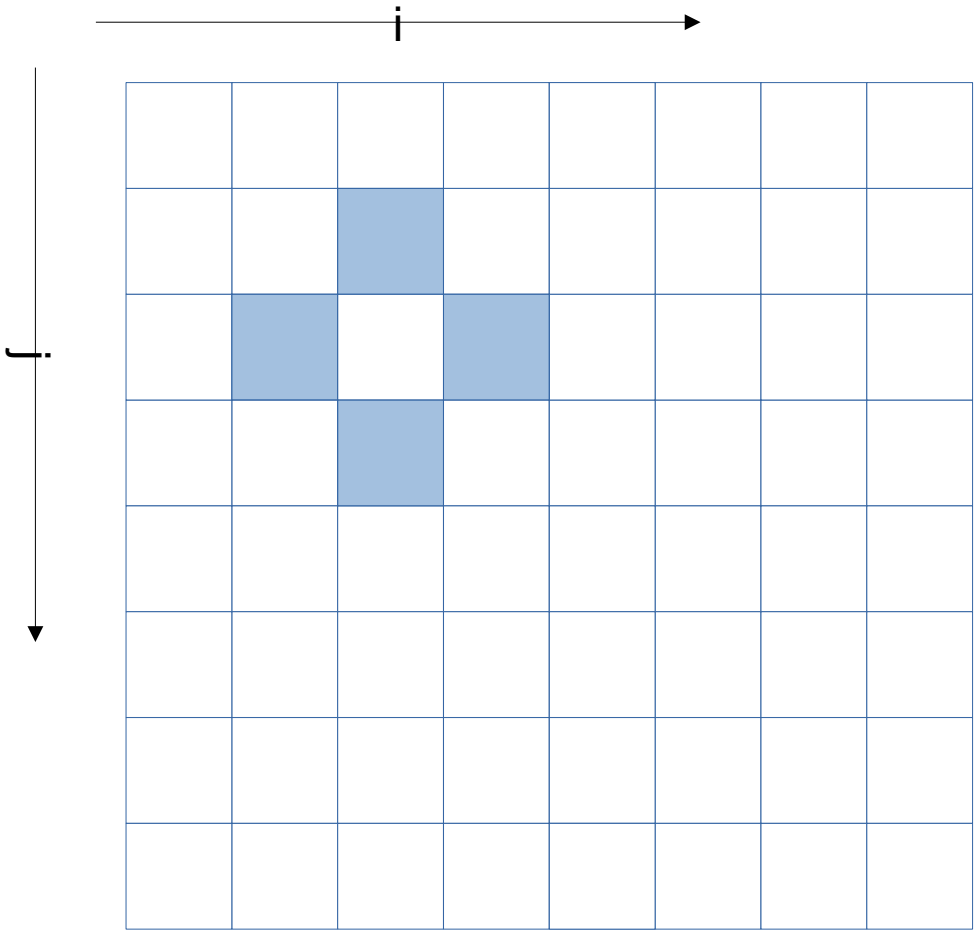
Loop is potentially data access bound.

Workaround

Unroll your loop if trip count is significantly higher than target unroll factor and if some data references are common to consecutive iterations. This can be done manually. Or by combining O2/O3 with the UNROLL (resp. UNROLL_AND_JAM) directive on top of the inner (resp. surrounding) loop. You can enforce an unroll factor: e.g. UNROLL(4).

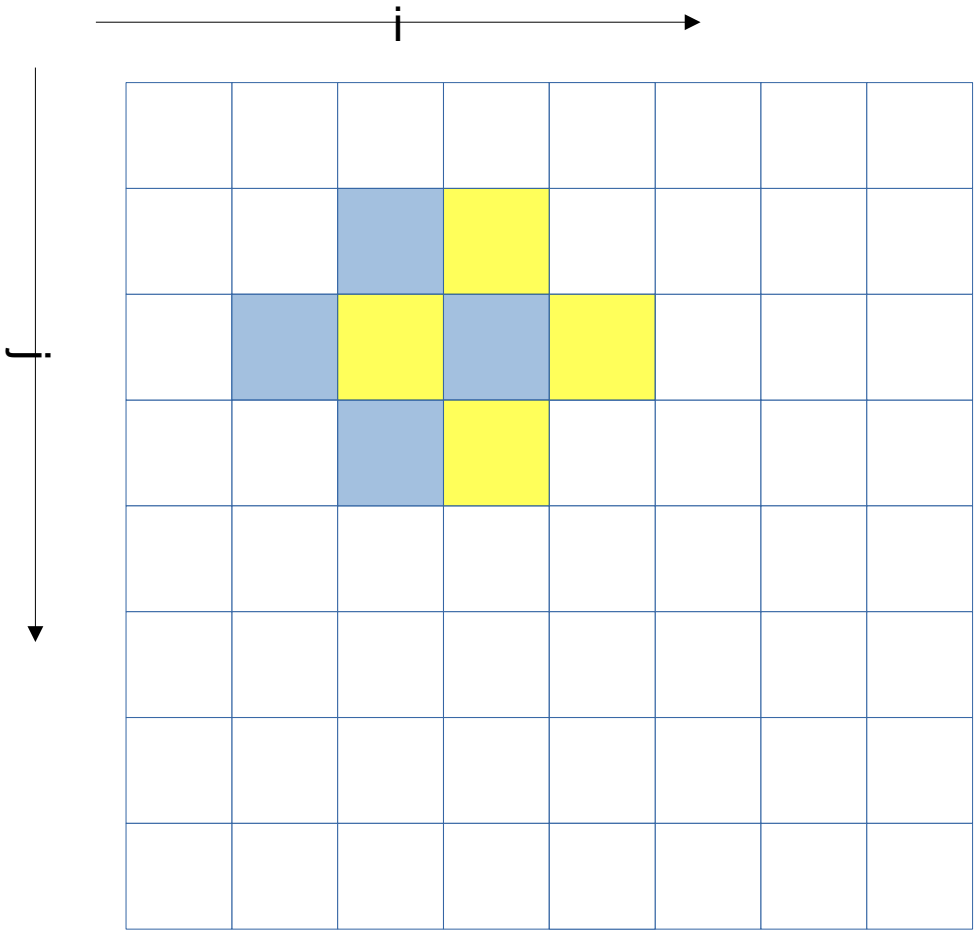
Unrolling is generally a good deal: fast to apply and often provides gain. Let's try to reuse data references through unrolling

Memory references reuse : 4x4 unroll footprint on loads



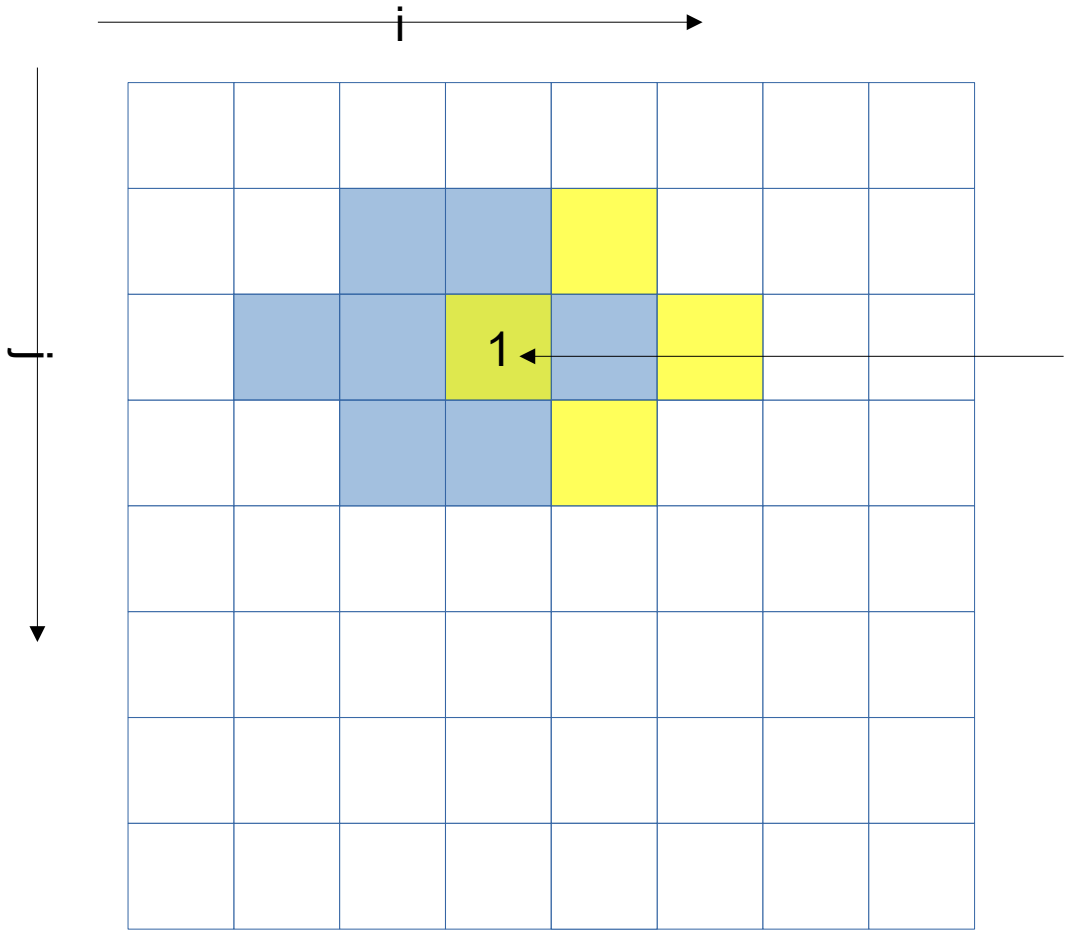
LINEAR_SOLVER(i+0,j+0)

Memory references reuse : 4x4 unroll footprint on loads



LINEAR_SOLVER(i+0,j+0)
LINEAR_SOLVER(i+1,j+0)

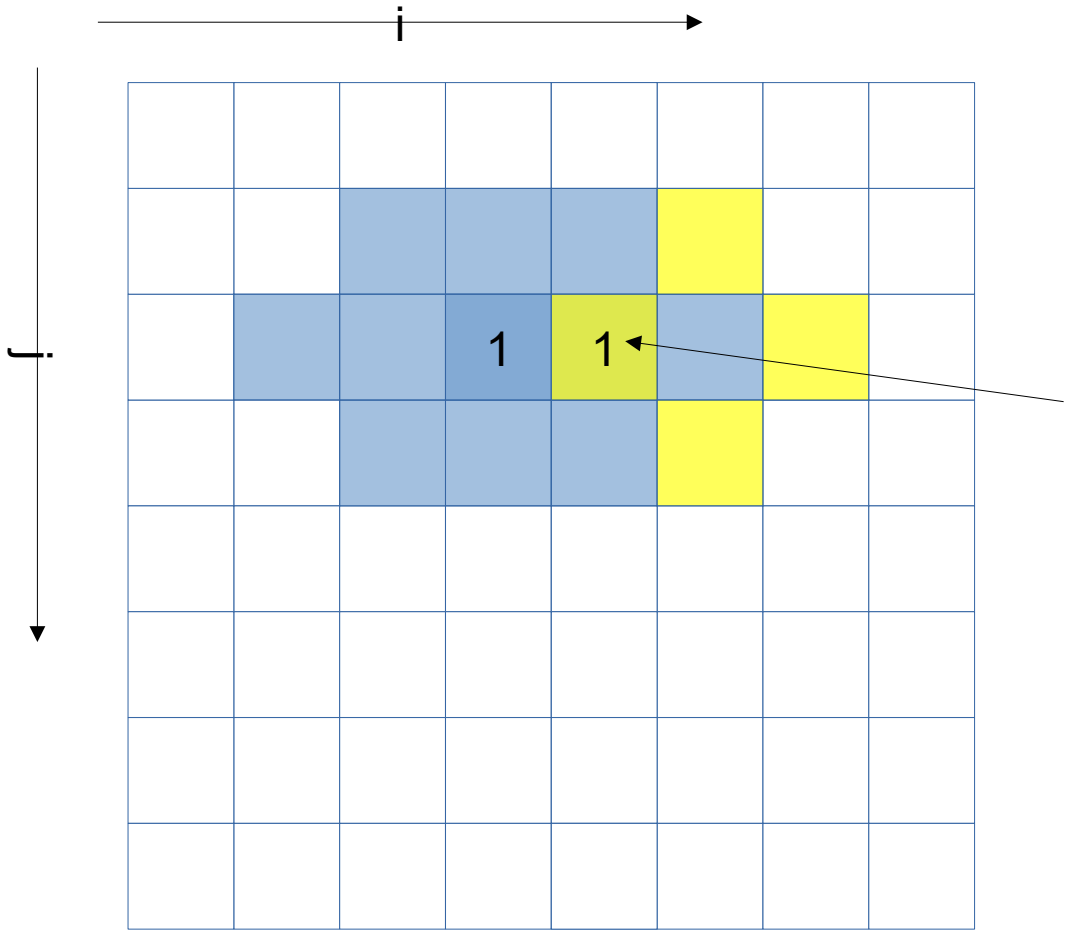
Memory references reuse : 4x4 unroll footprint on loads



LINEAR_SOLVER(i+0,j+0)
LINEAR_SOLVER(i+1,j+0)
LINEAR_SOLVER(i+2,j+0)

1 reuse

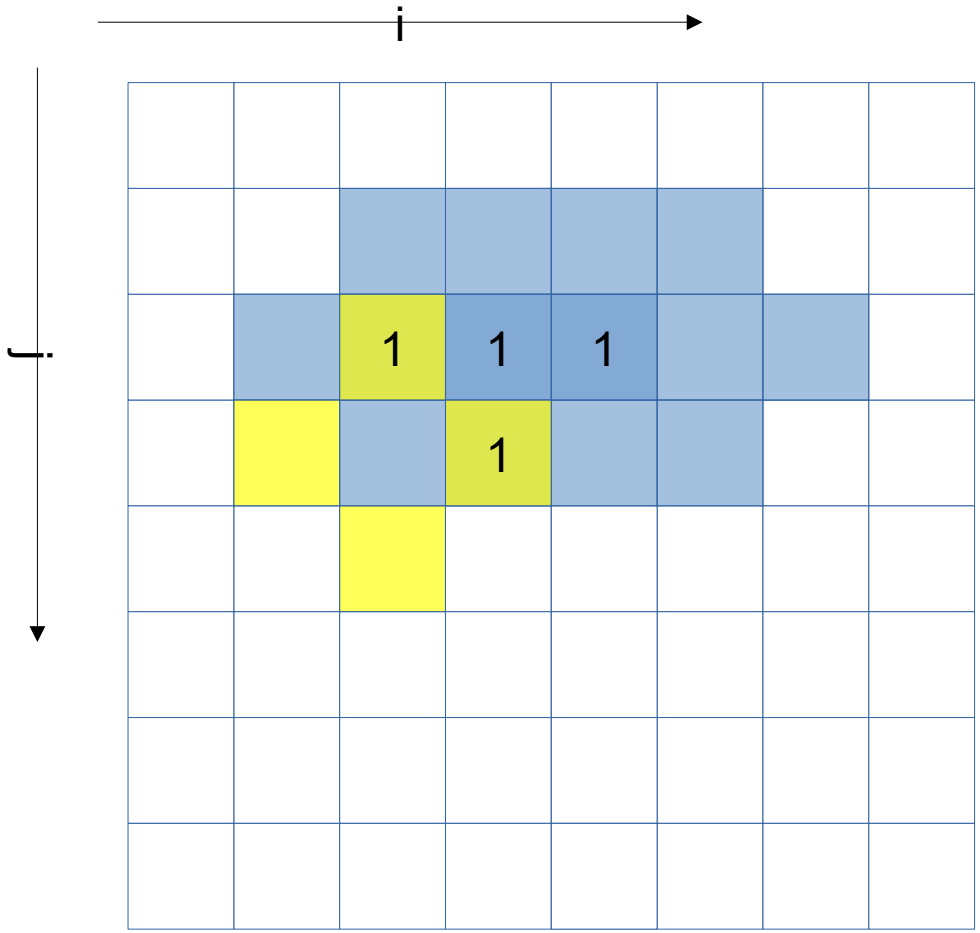
Memory references reuse : 4x4 unroll footprint on loads



LINEAR_SOLVER(i+0,j+0)
LINEAR_SOLVER(i+1,j+0)
LINEAR_SOLVER(i+2,j+0)
LINEAR_SOLVER(i+3,j+0)

2 reuses

Memory references reuse : 4x4 unroll footprint on loads

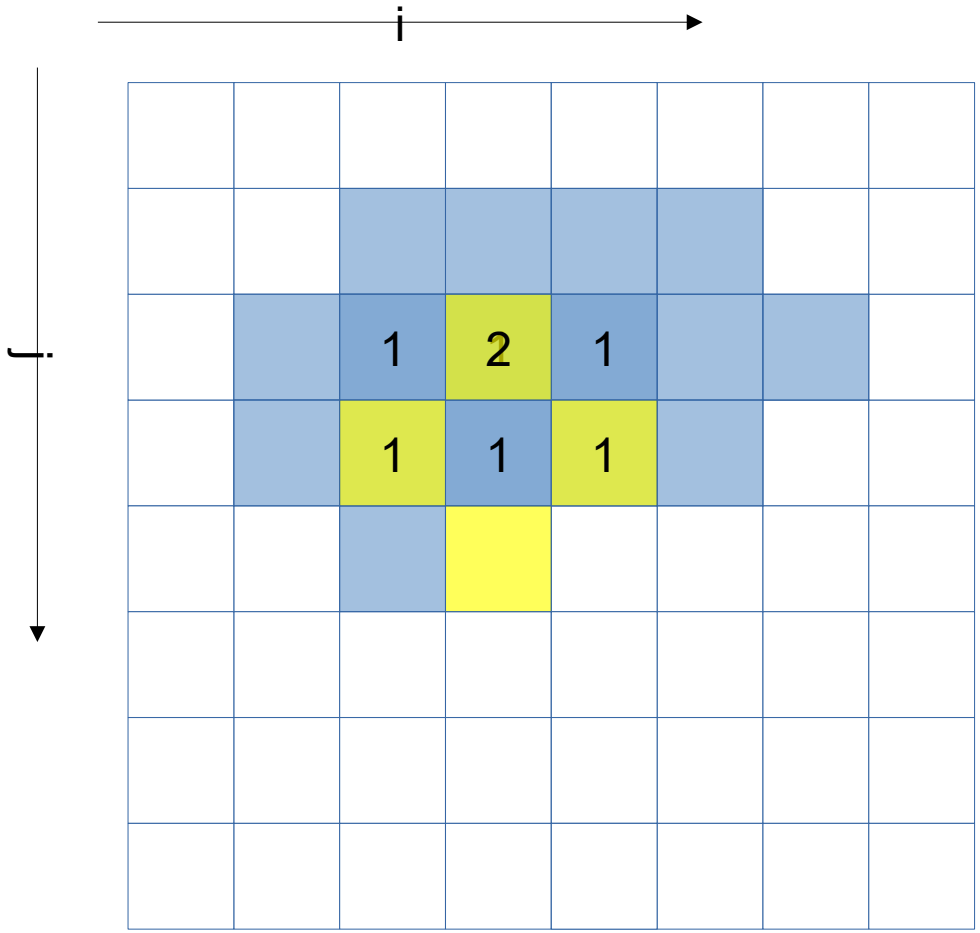


LINEAR_SOLVER(i+0,j+0)
LINEAR_SOLVER(i+1,j+0)
LINEAR_SOLVER(i+2,j+0)
LINEAR_SOLVER(i+3,j+0)

LINEAR_SOLVER(i+0,j+1)

4 reuses

Memory references reuse : 4x4 unroll footprint on loads

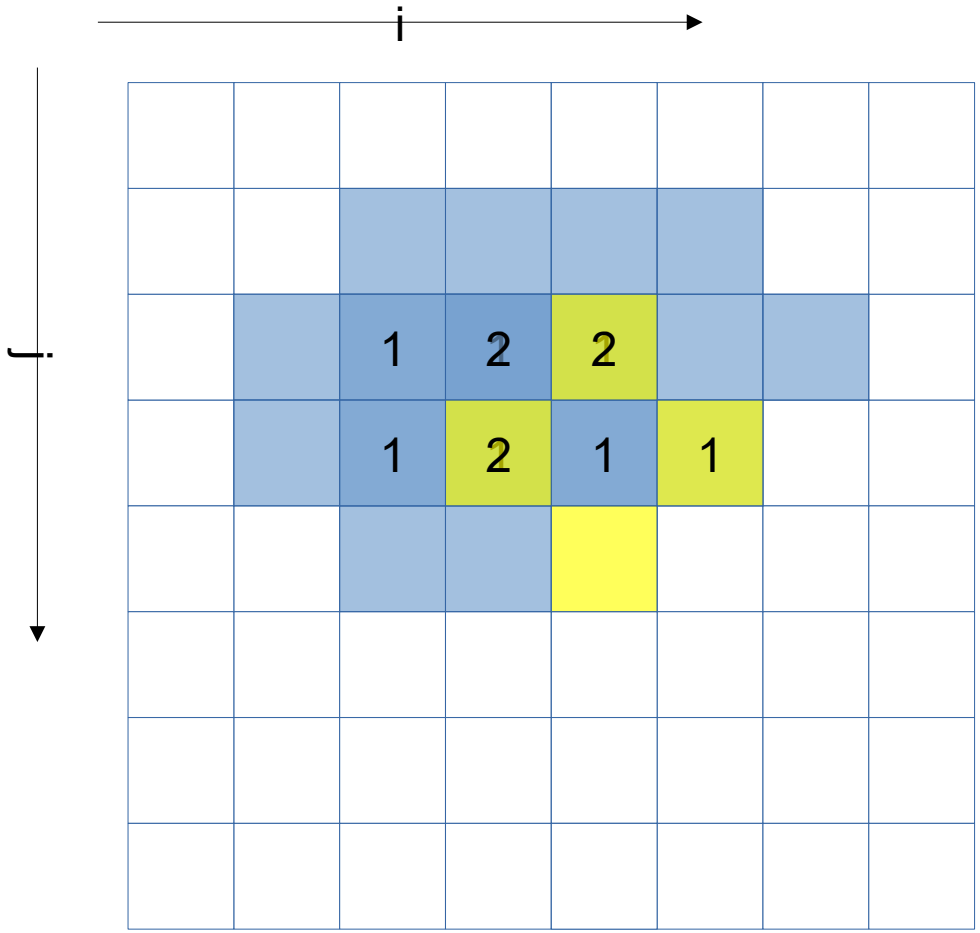


LINEAR_SOLVER(i+0,j+0)
LINEAR_SOLVER(i+1,j+0)
LINEAR_SOLVER(i+2,j+0)
LINEAR_SOLVER(i+3,j+0)

LINEAR_SOLVER(i+0,j+1)
LINEAR_SOLVER(i+1,j+1)

7 reuses

Memory references reuse : 4x4 unroll footprint on loads

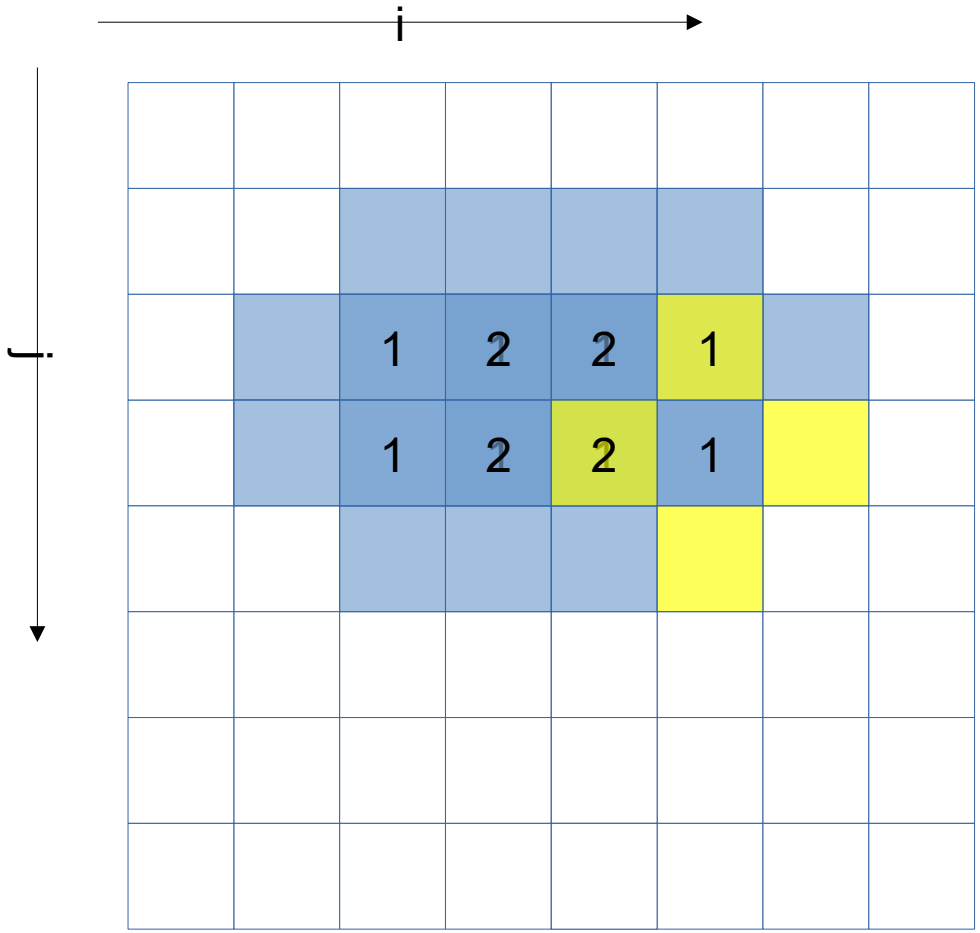


LINEAR_SOLVER(i+0,j+0)
LINEAR_SOLVER(i+1,j+0)
LINEAR_SOLVER(i+2,j+0)
LINEAR_SOLVER(i+3,j+0)

LINEAR_SOLVER(i+0,j+1)
LINEAR_SOLVER(i+1,j+1)
LINEAR_SOLVER(i+2,j+1)

10 reuses

Memory references reuse : 4x4 unroll footprint on loads

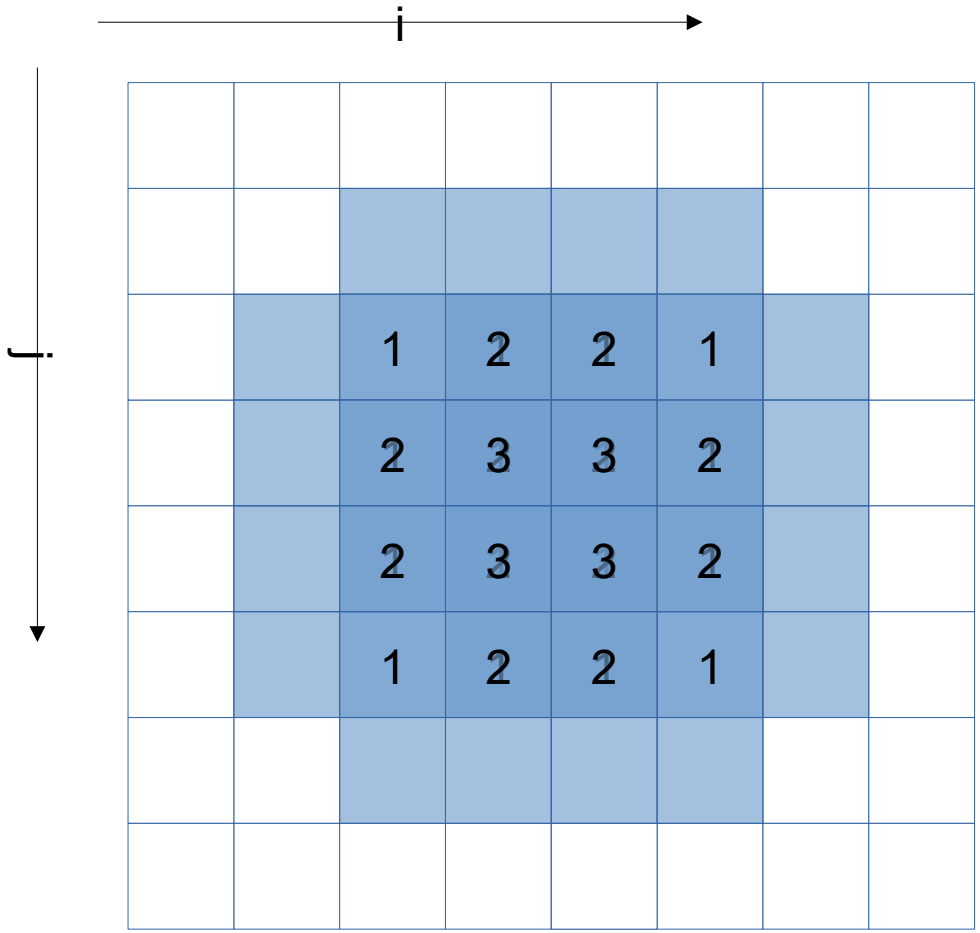


LINEAR_SOLVER(i+0,j+0)
LINEAR_SOLVER(i+1,j+0)
LINEAR_SOLVER(i+2,j+0)
LINEAR_SOLVER(i+3,j+0)

LINEAR_SOLVER(i+0,j+1)
LINEAR_SOLVER(i+1,j+1)
LINEAR_SOLVER(i+2,j+1)
LINEAR_SOLVER(i+3,j+1)

12 reuses

Memory references reuse : 4x4 unroll footprint on loads



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)

32 reuses

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 (...) {
  (...)

  for (k=0; k<20; k++)
    for (i=1; i<=grid_size-3; i+=4)
      for (j=1; j<=grid_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

Running and analyzing kernel1

Profile with MAQAO

```
> maqao oneview -R1 -xp=ov_k1 -c=ov_k1.lua
```

Viewing results (HTML)

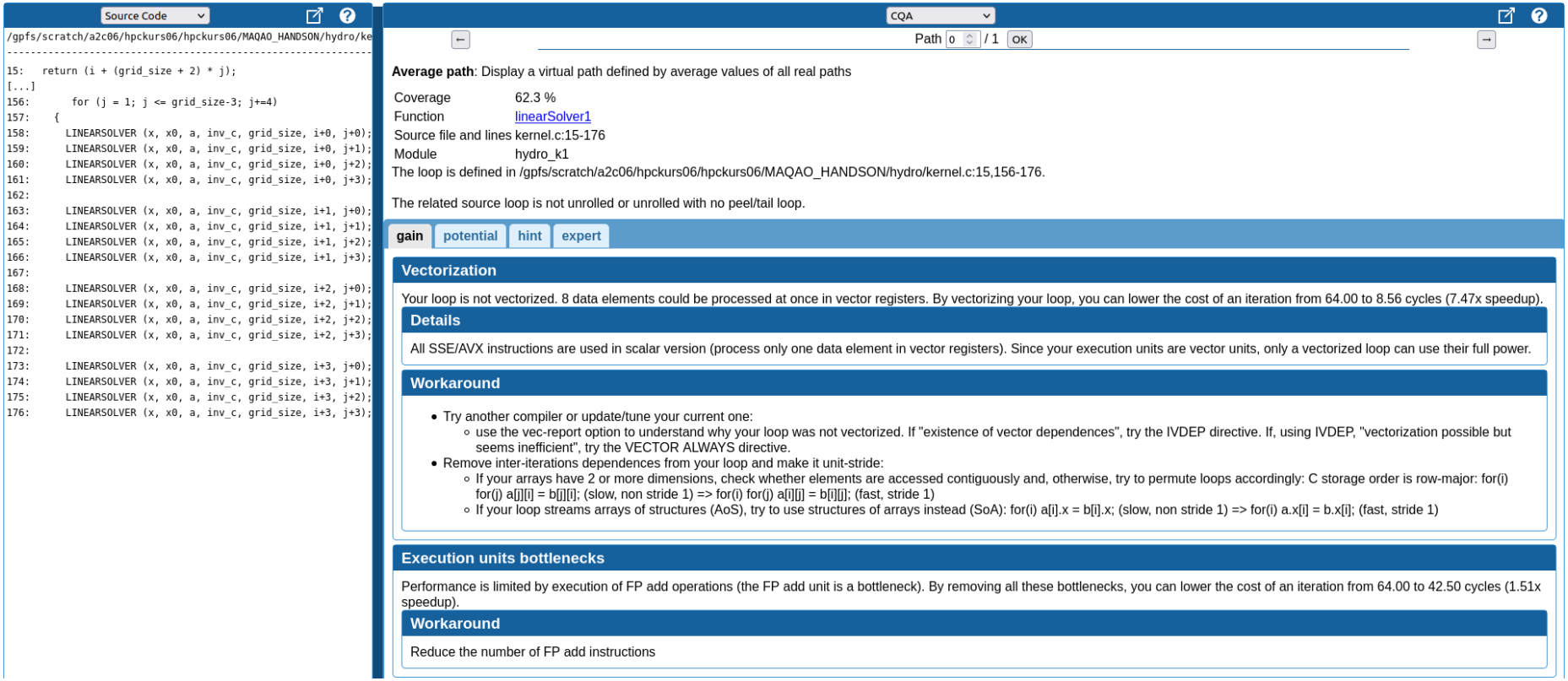
On your local machine (sshfs):

```
> firefox ivymuc_work/MAQAO_HANDSON/hydro/ov_k1/RESULTS/
hydro_k1_one_html/index.html &
```

Global Metrics

Total Time (s)		8.03
Profiled Time (s)		8.03
Time in loops (%)		99.92
Time in innermost loops (%)		99.88
Time in user code (%)		99.96
Compilation Options		OK
Perfect Flow Complexity		1.10
Array Access Efficiency (%)		53.66
Perfect OpenMP + MPI + Pthread		1.00
Perfect OpenMP + MPI + Pthread + Perfect Load Distribution		1.00
No Scalar Integer	Potential Speedup	1.01
	Nb Loops to get 80%	3
FP Vectorised	Potential Speedup	1.48
	Nb Loops to get 80%	3
Fully Vectorised	Potential Speedup	5.95
	Nb Loops to get 80%	8
FP Arithmetic Only	Potential Speedup	1.14
	Nb Loops to get 80%	8

Running and analyzing kernel1



CQA output for kernel1

Type of elements and instruction set

96 SSE or AVX instructions are processing arithmetic or math operations on single precision FP elements in scalar mode (one at a time).

Matching between your loop (in the source code) and the binary loop

The binary loop is composed of 96 FP arithmetical operations:

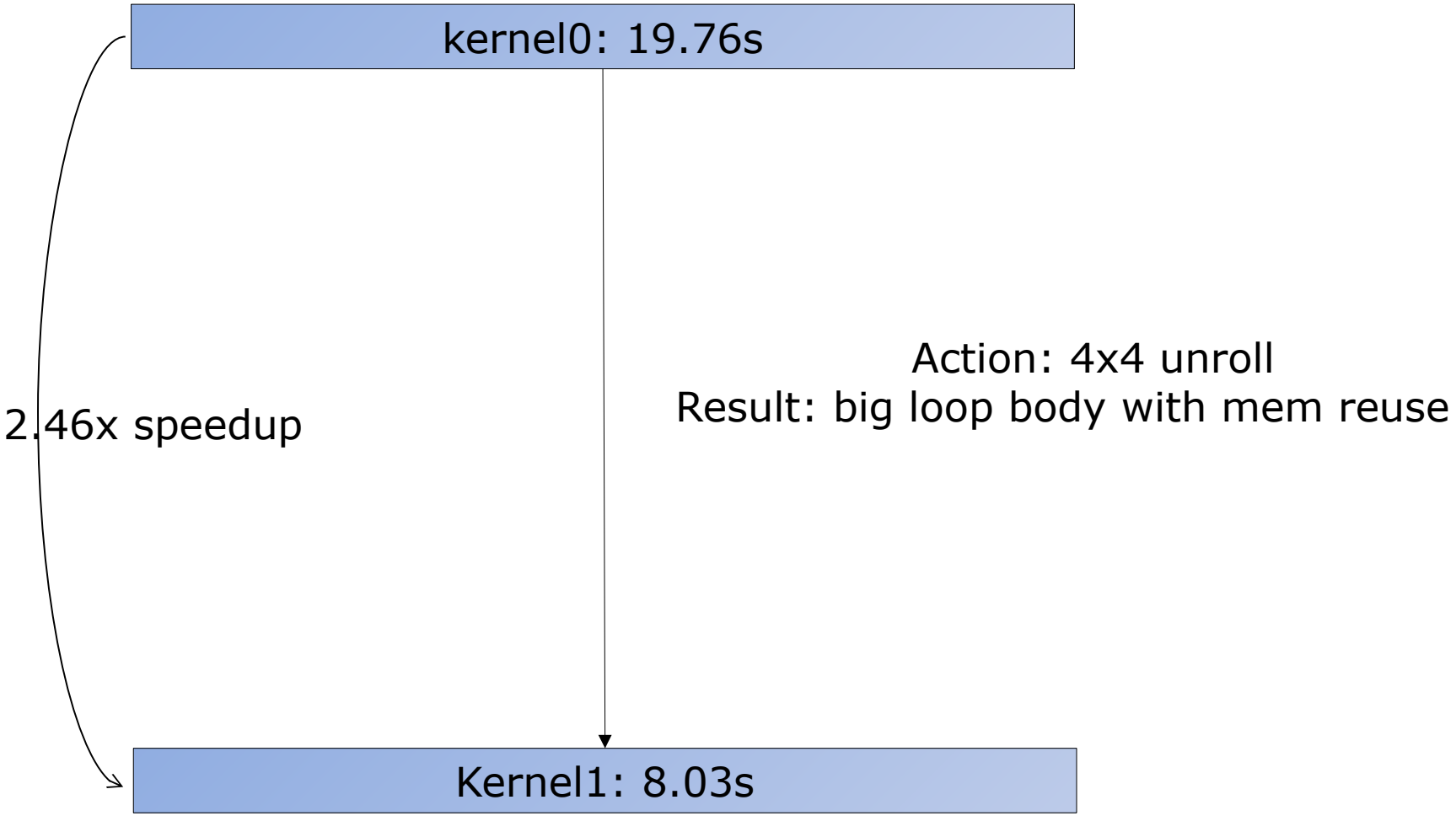
- 64: addition or subtraction
- 32: multiply

The binary loop is loading 276 bytes (69 single precision FP elements). The binary loop is storing 64 bytes (16 single precision FP elements).

4x4 Unrolling were applied

Expected 48... But still better than 80

Summary of optimizations and gains



More sample codes

More codes to study with MAQAO in

```
$WORK/MAQAO_HANDSON/loop_optim_tutorial.tgz
```

Scalability profiling of lulesh with MAQAO

Salah Ibnamar

Compiling Lulesh (on login node)

Copy Lulesh sources to your working directory

```
> cd $WORK
> tar xvf $TW40/material/maqao/lulesh2.0.3.tgz
```

(if necessary: reload Intel environment) Compile Lulesh

```
> cd lulesh
> module purge # if necessary
> module load admin/1.0 lrz/1.0 devEnv/Intel/2019 #if necessary
> make
```

(Optional) To execute a sample run of Lulesh:

```
> less job_lulesh.sbatch
> sbatch job_lulesh.sbatch
```

Setup ONE View for scalability analysis

Retrieve the configuration file prepared for lulesh in batch mode from the MAQAO_HANDSON directory

```
> cd $WORK/lulesh #if current directory has changed
> cp $WORK/MAQAO_HANDSON/lulesh/config_maqao_lulesh.lua .
> less config_maqao_lulesh.lua
```

```
binary = "./lulesh2.0"
...
run_command = "<binary> -i 10 -p -s 130"
...
batch_script = "job_lulesh_maqao.sbatch"
...
batch_command = "sbatch <batch_script>"
...
number_processes = 1
...
number_nodes = 1
...
mpi_command = "mpirun -n <number_processes>"
...
omp_num_threads = 1
...
multiruns_params = {
 {number_processes = 1, omp_num_threads =  8, number_nodes = 1, number_processes_per_node = 1},
 {number_processes = 8, omp_num_threads =  1, number_nodes = 1, number_processes_per_node = 8,
  run_command = "<binary> -i 10 -p -s 65"},
 {number_processes = 8, omp_num_threads =  1, number_nodes = 2, number_processes_per_node = 4...},
 {number_processes = 8, omp_num_threads =  4, number_nodes = 2, number_processes_per_node = 4...},
}
```

Review jobscript for use with ONE View

All variables in the jobscript defined in the configuration file must be replaced with their name from it.
Retrieve jobscript modified for ONE View from the MAQAO_HANDSON directory.

```
> cd $WORK/lulesh #if current directory has changed
> cp $WORK/MAQAO_HANDSON/lulesh/job_lulesh_maqao.sbatch .
> less job_lulesh_maqao.sbatch
```

```
...
#SBATCH --nodes=2<number_nodes>
...
export OMP_NUM_THREADS=8<omp_num_threads>
...
mpirun -n ... $EXE
<mpi_command> <run_command>
...
```

Launch MAQAO ONE View on lulesh (scalability mode)

Launch ONE View (execution will be longer!)

```
> module use $TW40/modulefiles
> module load maqao
> maqao oneview -R1 --with-scalability=on \
-c=config_maqao_lulesh.lua -xp=maqao_lulesh
```

The results can then be accessed similarly to the analysis report.

```
> firefox
ivymuc_work/lulesh/maqao_lulesh/RESULTS/lulesh2.0_one_html/index.html
```

OR

```
> tar czf $HOME/lulesh_html.tgz \
maqao_lulesh/RESULTS/lulesh2.0_one_html
```

```
> scp <user>@lxlogin10.lrz.de:lulesh_html.tgz .
> tar xf lulesh_html.tgz
> firefox maqao_lulesh/RESULTS/lulesh2.0_one_html/index.html
```

A sample result directory is in **MAQAO_HANDSON/lulesh/lulesh_html_example.tgz**