Shallow Water Simulation

CS 5220: Homework 2

Group 1

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1 Profiling

We refer to the use profiling tools on the note "Optimization and analysis tools".

1.1 VTune Amplifier

We can use the command line interface amplxe-cl to run the VTune GUI from our head node. The collection phase will run on the compute nodes in the cluster. Once the data has been collected, reports can be generated on the front-end node.

1.1.1 C++ Code

We first used amplxe to get profiling result of the C++ code. From the report below, we find out that we should give our priority to improving functions limited_derivs, compute_step and compute_fg_speeds in Central2D, because they take the majority of CPU time.

Function	Module	CPU Time
${\tt Central2D < Shallow2D} \;, \; \; {\tt MinMod < float >> :: limited_derivs}$	shallow	$1.356\mathrm{s}$
${\tt Central2D < Shallow2D}\;,\;\; {\tt MinMod < float} >> :: {\tt compute_step}$	shallow	$0.642\mathrm{s}$
$Central 2D < Shallow 2D\;,\;\; MinMod < \verb float >> :: compute_fg_speeds $	shallow	$0.229\mathrm{s}$

_IO_fwrite	libc-2.12.so	$0.023\mathrm{s}$
[Outside any known module]	$[\mathrm{Unknown}]$	$0.019\mathrm{s}$
_IO_file_xsputn	libc-2.12.so	$0.014\mathrm{s}$
$Central 2D < Shallow 2D \;, \; \; MinMod < \texttt{float} >> :: \texttt{solution_check}$	shallow	$0.007\mathrm{s}$
$\label{low2D} SimViz < Central 2D < Shallow 2D \;, \; \; MinMod < \texttt{float} >> :: write_frame$	shallow	$0.005\mathrm{s}$
$Central 2D < Shallow 2D \;,\;\; MinMod < \texttt{float} >> :: run$	shallow	$0.003\mathrm{s}$
Central2D <shallow2d. minmod<float="">>::offset</shallow2d.>	shallow	$0.002 \mathrm{s}$

1.1.2 C Code

Unfortunately, later when we are trying to profile with the C version with amplxe, we found that it was down due to some unknown issues. We found other groups experiencing the same issues. So instead, we used MAQAO as our profiling tools.

1.2 Modular Assembly Quality Analyzer and Optimizer (MAQAO)

MAQAO is a relatively new tool that provides detailed analysis of the shortcomings of our code based on a static analysis of the generated assembly language. Unfortunately, MAQAO does not provide timing results. We leave the comparison of timing results before/after tuning in the following sections.

1.2.1 C++ Code

We first present the MAQAO output for the plain C++ code. From the report below, we know that we should give priority to improving function compute_step in Central2D, since it is the most problematic and promising one.

Section 1: Function: Central2D<Shallow2D, MinMod<float> >::compute_step(int, float)

Section 1.1: Source loop ending at line 338

Pathological cases

Your loop is processing FP elements but is NOT OR PARTIALLY VECTORIZED

and could benefit from full vectorization.

Since your execution units are vector units, only a fully vectorized loop can use their full power.

By fully vectorizing your loop, you can lower the cost of an iteration from 13.25 to 3.18 cycles (4.17x speedup).

Two propositions:

- Try another compiler or update/tune your current one:
 - * Intel: use the vec-report option to understand why your loop was not vectorized.

If "existence of vector dependences", try the IVDEP directive. If, using IVDEP,

- "vectorization possible but seems inefficient", try the VECTOR ALWAYS directive.
- Remove inter-iterations dependences from your loop and make it unit-stride.

Detected EXPENSIVE INSTRUCTIONS, generating more than one micro-operation.

Only one of these instructions can be decoded during a cycle and the extra micro-operations increase pressure on execution units.

VCVTSD2SS: 2 occurrences

VCVTSS2SD: 3 occurrences

- Pass to your compiler a micro-architecture specialization option:
 - * Intel: use axHost or xHost.

Fix as many pathological cases as you can before reading the following sections.

${\tt Bottlenecks}$

The ROB-read stage is a bottleneck.

By removing all these bottlenecks, you can lower the cost of an iteration from 13.25 to 12.00 cycles (1.10x speedup).

Section 1.2: Source loop ending at line 357

Pathological cases

Your loop is processing FP elements but is NOT OR PARTIALLY VECTORIZED and could benefit from full vectorization.

Since your execution units are vector units, only a fully vectorized loop can use their full power.

By fully vectorizing your loop, you can lower the cost of an iteration from 54.00 to 7.50 cycles $(7.20 \times \text{speedup})$.

Two propositions:

- $-\ \mathrm{Try}$ another compiler or update/tune your current one:
- * Intel: use the vec-report option to understand why your loop was not vectorized.

If "existence of vector dependences", try the $\overline{\text{IVDEP}}$ directive. If, using $\overline{\text{IVDEP}}$,

"vectorization possible but seems inefficient", try the VECTOR ALWAYS directive.

- Remove inter-iterations dependences from your loop and make it unit-stride.

Detected EXPENSIVE INSTRUCTIONS, generating more than one micro-operation.

Only one of these instructions can be decoded during a cycle and the extra micro-operations increase pressure on execution units.

VCVTSD2SS: 3 occurrences

VCVTSS2SD: 12 occurrences

- Pass to your compiler a micro-architecture specialization option:
 - * Intel: use axHost or xHost.

Fix as many pathological cases as you can before reading the following sections.

Bottlenecks

The FP add unit is a bottleneck.

Try to reduce the number of FP add instructions.

By removing all these bottlenecks, you can lower the cost of an iteration from 54.00 to 40.50 cycles (1.33x speedup).

Section 1.3: Source loop ending at line 364

Pathological cases

Your loop is processing FP elements but is NOT OR PARTIALLY VECTORIZED and could benefit from full vectorization.

Since your execution units are vector units, only a fully vectorized loop can use their full power.

By fully vectorizing your loop, you can lower the cost of an iteration from 3.00 to 0.75 cycles $(4.00 \times \text{speedup})$.

Two propositions:

- Try another compiler or update/tune your current one:
 - * Intel: use the vec-report option to understand why your loop was not vectorized.

If "existence of vector dependences", try the IVDEP directive. If, using IVDEP,

- "vectorization possible but seems inefficient", try the VECTOR ALWAYS directive.
- Remove inter-iterations dependences from your loop and make it unit-stride.

Fix as many pathological cases as you can before reading the following sections.

Bottlenecks

The store unit is a bottleneck.

Try to reduce the number of stores.

For example, provide more information to your compiler:

- hardcode the bounds of the corresponding 'for' loop,

By removing all these bottlenecks, you can lower the cost of an iteration from 3.00

```
to 2.25 cycles (1.33x speedup).
```

1.2.2 C Code

We also consider the following profiling results of C code by Professor Bindel using MAQAO. As Professor Bindel mentioned, the C code is highly vectorized and there is very little room for improvement in terms of serial performance. We leave this topic in subsequent sections. We present here part of result of *step* function that we found most problematic in C++ version. In C version, loops are almost fully vectorized and the performance boost is obvious.

Section 2: Function: central2d_step

```
These loops are supposed to be defined in: \frac{\protect}{\protect} \protect}{\protect} 162 Section 2.1: Source loop ending at line 162
```

```
Composition and unrolling
```

```
It is composed of the following loops [ID (first-last source line)]:

- 49 (133-162)

- 50 (133-162)

and is unrolled by 8 (including vectorization).

The following loops are considered as:

- unrolled and/or vectorized: 50

- peel or tail: 49, 51

The analysis will be displayed for the unrolled and/or vectorized loops: 50

Section 2.1.1: Binary (unrolled and/or vectorized) loop #50
```

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

Type of elements and instruction set

 $^{9~\}mathrm{AVX}$ instructions are processing arithmetic or math operations on single precision FP elements in vector mode (eight at a time). Vectorization

Your loop is fully vectorized (all SSE/AVX instructions are used in vector mode and on full vector length).

The binary loop is composed of 56 FP arithmetical operations:

- 40: addition or subtraction
- 16: multiply

The binary loop is loading 96 bytes (24 single precision FP elements).

The binary loop is storing 32 bytes (8 single precision FP elements).

Arithmetic intensity is 0.44 FP operations per loaded or stored byte.

Cycles and resources usage

Assuming all data fit into the L1 cache, each iteration of the binary loop takes 12.00 cycles. At this rate:

- 14% of peak computational performance is reached (4.67 out of 32.00 FLOP per cycle (GFLOPS @ 1GHz))
- 12% of peak load performance is reached (8.00 out of 64.00 bytes loaded per cycle (GB/s @ 1GHz))
- 8% of peak store performance is reached (2.67 out of 32.00 bytes stored per cycle (GB/s @ 1GHz))

Pathological cases

None detected.

Bottlenecks

The P5 port or a related execution unit is a bottleneck.

By removing all these bottlenecks, you can lower the cost of an iteration from 12.00 to 7.00 cycles (1.71x speedup).

2 Parallelization

We use OpenMP to parallelize our code, and start with a naive parallelization (e.g. parallelizing the for loops in the various subroutines).

2.1 C++ Code

2.1.1 limited_derivs

We apply the parallel region and for directive.

template <class Physics, class Limiter>

2.1.2 limited_derivs

We rewrite the two-for loop as one-for loop, then apply the parallel region and for directive.

2.1.3 limited_derivs

We apply the parallel region and sections directive.

```
template <class Physics, class Limiter>
void Central2D<Physics , Limiter >::limited_derivs()
    int iy, ix;
    #pragma omp parallel private(iy, ix)
        for (iy = 1; iy < ny_all_{-1}; ++iy)
             for (ix = 1; ix < nx_all -1; ++ix) {
                 #pragma omp sections
                     #pragma omp section
                     // x derivs
                     . . .
                     #pragma omp section
                     // y derivs
                     . . .
                 }
            }
    }
}
```

2.1.4 compute_step

We apply the parallel region and for directive for two blocks.

```
#pragma omp for

// Corrector (finish the step)

for (iy = nghost-io; iy < ny+nghost-io; ++iy)

    for (ix = nghost-io; ix < nx+nghost-io; ++ix) {

        for (m = 0; m < v(ix,iy).size(); ++m) {

            ...

        }

    }

// Copy from v storage back to main grid
...
}</pre>
```

See Figure 1 and 2 below for strong and weak studies, where two-layer for in limited_derivs + for in compute_step corresponds to version 1, and one-layer for in limited_derivs + for in compute_step corresponds to version 2.

2.2 C Code

2.2.1 barrier

We apply the parallel region and barrier directive for two blocks.

```
int central2d_xrun(float* restrict u, ..., int nx, ..., int nthread, int nbatch)
{
  int nstep = 0;
  float t = 0;
  ...

// allocate memory for block cells

while (!done) {
    // check whether it is done

#pragma omp parallel num_threads(nthread)
    {
```

```
int thread_id = omp_get_thread_num();
         // copy to block cells
         \quad \text{for(int } k = 0; \ k < \text{nfield;} +\!\!\!+\!\! k) \ \{
              memcpy(u\_block[thread\_id]+k*nx\_all*(2*nbatch+block\_size),
              u + k*n x\_all*n y\_all + n x\_all*(\ block\_size*thread\_id\ )\ ,
              nx_all*(2*nbatch+block_size)*sizeof(float));
         }
         #pragma omp barrier
         // compute block cells
         \label{eq:for_int} \text{for}\,(\,\text{int}\ j\ =\ 0\,;\ j\ <\ \text{nbatch}\ /\ 2\,;\ +\!\!\!+\!\!\!j\,)\ \{
              // 1st step
              central2d_step(u_block[thread_id], ..., 0, ...);
              // 2nd step
              central2d_step(u_block[thread_id], ..., 1, ...);
         }
         // copy from block cells
         for (int k = 0; k < n field; ++k) {
              memcpy(u+k*nx_all*ny_all+nx_all*(ng+block_size*thread_id),
               u\_block [thread\_id] + k*nx\_all*(2*nbatch+block\_size) + nbatch*nx\_all , \\
              nx_all*block_size*sizeof(float));
         }
         #pragma omp barrier
    }
    // update t and nstep
    t += nbatch * dt;
    nstep += nbatch;
}
// free memory for block cells
for (int i = 0; i < nthread; ++i) {
     free(u_block[i]);
```

```
return nstep;
```

See Figure 3 and 4 below for strong and weak studies, where domain decomposition corresponds to version 2.

3 Tuning

Given the profiling results presented above, we consider the following aspects of tuning.

3.1 Vectorization

3.1.1 C++ code

We first considered if we can vectorize C++ code as much as possible. By using the compiler flag

```
\texttt{-qopt-report-phase=vec -qopt-report=5 -qopt-report-file=stdout}
```

we get a detailed vectorization report including information such as which loops are vectorized and why certain loops are note. For example, from amplxe report we know that another function we need to tune is compute_fg_speeds. The vectorization report about this function is as follows.

```
Begin optimization report for: Central2D<Shallow2D, MinMod<Shallow2D::real>>::compute_fg_speeds(Central2D<Shallow2D, MinMod<Shallow2D::real>>::real>>::real &, Central2D<Shallow2D, MinMod<Shallow2D::real>>::real &)

Report from: Vector optimizations [vec]

LOOP BEGIN at central2d.h(267,5)

remark #15344: loop was not vectorized: vector dependence prevents vectorization
```

```
remark #15346: vector dependence: assumed FLOW dependence between _M_elems line 74

and _M_elems line 76

remark #15346: vector dependence: assumed ANTI dependence between _M_elems line 76

and _M_elems line 74

LOOP BEGIN at central2d.h(268,9)

remark #15344: loop was not vectorized: vector dependence prevents vectorization

remark #15346: vector dependence: assumed FLOW dependence between _M_elems line 74

and _M_elems line 76

remark #15346: vector dependence: assumed ANTI dependence between _M_elems line 76

and _M_elems line 74

LOOP END

LOOP END
```

Note that the compiler assumes multiple FLOW and ANTI dependencies that prevent the loop from being vectorized. However, this function is basically doing copy from one vector to another, which inherently should be able to get vectorized. To resolve dependencies, we first used the annotation #pragma ivdep. As suggested by the output of MAQAO, using this annotation might be able to resolve incorrectly assumed dependency in loops in some cases.

```
template <class Physics, class Limiter>
void Central2D<Physics, Limiter>::compute_fg_speeds(real& cx_, real& cy_)
{
    using namespace std;
    real cx = 1.0e-15;
    real cy = 1.0e-15;
    #pragma ivdep
    for (int iy = 0; iy < ny_all; ++iy)
        for (int ix = 0; ix < nx_all; ++ix) {
            real cell_cx , cell_cy;
            Physics:: flux(f(ix, iy), g(ix, iy), u(ix, iy));
            Physics::wave_speed(cell_cx, cell_cy, u(ix,iy));
            cx = max(cx, cell_cx);
            cy = max(cy, cell_cy);
        }
    cx_{-} = cx;
    cy_- = cy;
```

}

See Figure 5 and 6 for strong and weak studies with #pragma ivdep

The vectorization report after using this annotation gives positive result

```
remark #15300: LOOP WAS VECTORIZED

remark #15460: masked strided loads: 6

remark #15462: unmasked indexed (or gather) loads: 6

remark #15475: — begin vector loop cost summary —

remark #15476: scalar loop cost: 308

remark #15477: vector loop cost: 76.870

remark #15478: estimated potential speedup: 3.840

remark #15479: lightweight vector operations: 109

remark #15481: heavy—overhead vector operations: 1

remark #15487: type converts: 8

remark #15488: — end vector loop cost summary —
```

gives a potential speed up around 3.840.

Figures 7 and 8 show the results when we add #pragma simd and #ivdep in certain chunks. However, adding annotations like this and some others like #pragma simd, #pragma always vectorize and #pragma omp declare simd are not guaranteed to successively vectorize every loop.

The potential reason behind might be the fact that the data structure used to represent a solution vector in the C++ code is inherently not amenable for vectorization. Note that by definition in shallow2d.h, solution vectors are std::vector of std::array. In specific, the instance vector $\mathbf{U}_1 = (u_1, hu_1, hv_1)$, $\mathbf{U}_2 = (u_2, hu_2, hv_2)$ and $\mathbf{U}_3 = (u_3, hu_3, hv_3)$ are in memory in the following sequence

$$u_1, hu_1, hv_1, u_2, hu_2, hv_2, u_3, hu_3, hv_3$$

However in most computations there is only one component of the array of size 3 is used. This is in turn bad in memory locality and is very hard for compiler to achieve vectorization accordingly.

We also consider rewriting the data structure that is more amenable to memory locality. In specific, the ideal memory layout should be of the pattern

$$u_1, u_2, u_3, hu_1, hu_2, hu_3, hv_1, hv_2, hv_3$$

Yet changing this means rewriting basically every implementation. Later we found the C code by Professor Bindel, which is highly vectorized. So we decided to continue our work based on the C version instead.

3.1.2 C code

Since the data structure issue discussed above no long exists in C code, we were playing around with annotations trying to get some bonus performance improvement. As the results shown below, there is very limited room for further improvement on the well-written C code. Great job Professor Bindel!

See Figure 9,10 for C code with annotations #pragma ivdep.

3.2 Offload

The totient cluster node (host) can offload work by directing the Xeon Phi accelerator boards (MIC) to execute a specified block of code. The host also directs the exchange of data between host and MIC.

There are three models of offload, explicit offload, implicit offload, and automatic offload. We mainly refer to the "Intel Xeon Phi MIC Offload Programming Models" by Doug James to implement them for the C code.

3.2.1 Explicit Offload

The explicit offload is one of compiler assisted offload, where we explicitly directs data movement and code execution by using #pragma offload target(mic).

Moreover, we need to specify the functions which host will share with MIC by using __attribute__((target(mic))), and specify the variables which host will share with MIC by using in(), out(), inout().

When we implement the explicit offload, we refer to the repository of Group 3 as well.

3.2.2 Implicit Offload

The explicit offload is another one of compiler assisted offload, where we mark some data as "shared" in the virtual sense, and automatically synchronizes values between host and MIC by using #pragma offload target(mic).

```
int _Cilk_shared central2d_xrun(float* restrict u, int nx, ...) {
```

```
int _Cilk_offload central2d_run(float* restrict u, int nx, ...)
{
  int _Cilk_shared nstep = 0;
  float* restrict _Cilk_shared u;

  nstep = central2d_xrun(u, nx, ...);

  return nstep;
}
```

3.2.3 Automatic Offload

The automatic offload makes computationally intensive calls to Intel Math Kernel Library (MKL), which automatically manages details.

We need to include the library <mkl.h> in our code and add the flag -mkl when we compile the code.

```
#include <mkl.h>
icc ... -openmp -mkl stepper.c
```

Also we need to set three environment variables before launching our code.

```
export MKL_MIC_ENABLE=1
export OMP_NUM_THREADS=16
export MIC_OMP_NUM_THREADS=240
```

See Figure 11 and 12 below for strong and weak studies, where domain decomposition corresponds to version 2, and domain decomposition + automatic offload corresponds to version 7.

3.3 Compiler flags

From the experience of last project, we understand that compiler flags sometime give really impressive performance gain. In serial code, we consider the following compiler flags

```
-03 -no-prec-div -xcore-avx2 -ipo
-qopt-report=5 -qopt-report-phase=vec
-axCORE-AVX512,CORE-AVX2
-unroll-aggressive -fp-model -fast
-restrict -openmp -ansi-alias -opt-prefetch -ftree-vectorize
```

Unfortunately, compiler flags give performance gain neither in C or C++ code. Possible reason might be again that C code has been highly vectorized while C++ code inherently is not amenable for further optimization.

See the following Figure 13-16 for the results with the above compiler flags together with annotations in C and C++ codes respectively.

In addition, we could add a specific flag -offload-attribute-target=mic for offload.

3.4 Domain decomposition

We divide all cells into a couple of blocks, and each block holds several layers of ghost cells in order to avoid frequent synchronization.

Basically, we denote the number of cells on one side by ncell, the number of threads by nthread, the number of frames by nframe, and the number of batches by nbatch. As a result, each thread computes a block, with the number of cells on one side ncell/nthread, and the layer of ghost cells on one side nframe/nbatch. Ideally, we could have both ncell/nthread and nframe/nbatch as integers in case studies.

When we implement the explicit offload, we refer to the repository of Group 17 as well.

In each step, we first allocate memory for block cells and copy original cells to block cells using malloc and memory, and then compute block cells based on the ghost cells, and finally copy block cells back to original cells.

```
// allocate memory for block cells
float** f-block = (float**) malloc(nthread*sizeof(float*));
```

```
for (int i = 0; i < nthread; ++i) {
    u_block[i] = (float*) malloc(nx_all*nfield*(2*nbatch+block_size)*sizeof(float));
}
// copy to block cells
for (int k = 0; k < nfield; ++k) {
    memcpy(\,u\_block\,[\,thread\_id\,] + k*nx\_all*(2*nbatch+block\_size\,)\,,
    u+k*nx_all*ny_all+nx_all*(block_size*thread_id),
    nx_all*(2*nbatch+block_size)*sizeof(float));
}
// compute block cells
for (int j = 0; j < nbatch / 2; ++j) {
    // 1st step
    central2d_step(u_block[thread_id], ..., 0, ...);
    // 2nd step
    central2d\_step(u\_block[thread\_id], \ldots, 1, \ldots);
}
// copy from block cells
for (int k = 0; k < n field; ++k) {
    memcpy(u+k*nx_all*ny_all+nx_all*(ng+block_size*thread_id),
    u_block[thread_id]+k*nx_all*(2*nbatch+block_size)+nbatch*nx_all,
    nx_all*block_size*sizeof(float));
}
```

4 Performance

We set up both strong and weak scaling studies, varying the number of threads we employ.

4.1 Strong Scaling Study

We fix the number of cells per side nx = 200 and vary the number of threads $p = 1^2, \dots, 8^2$. Therefore, the total number of cells is nx^2 , which does not change as the number of threads p changes.

The x-axis in all the plots should be \sqrt{p} .

According to Amdahl's law, we have the speedup as

$$S(p) = \frac{T_{\text{serial}}}{T_{\text{parallel}}(p)} = \frac{1}{\alpha + (1-\alpha)p} \le \frac{1}{\alpha}$$

where α is the fraction of the serial work.

4.2 Weak Scaling Study

We vary both the number of cells per side $nx = 200 \times p$ and the number of threads $p = 1^2, \dots, 8^2$. Therefore, the total number of cells is nx^2 , which is proportional to the number of threads p.

The x-axis in all the plots should be \sqrt{p} .

According to Gustafson's law, we have the speedup as

$$S(p) = \frac{T_{\text{serial}}(n(p))}{T_{\text{parallel}}(n(p),p)} = \frac{1}{\alpha + (1-\alpha)p} \le \frac{a+bp}{a+b} = p - \alpha(p-1)$$

where $\alpha = a/(a+b)$ is the fraction of serial work.

Reference

- (1) D. Bindel, Shallow water simulation, Applications of Parallel Computers (CS 5220), Fall 2015.
- (2) D. Bindel, Optimization and analysis tools, Applications of Parallel Computers (CS 5220), Fall 2015.
- (3) D. Bindel, Shallow Water Simulation, https://github.com/dbindel/water, 2015.
- $(4) \ B. \ Barney, \ Open MP, \ https://computing.llnl.gov/tutorials/open MP.$

- (5) D. James, Intel Xeon Phi MIC Offload Programming Models, https://portal.tacc.utexas.edu/documents/13601/901837/offload_slides_DJ2013-3.pdf.
- (6) G. Jiang and E. Tadmor, Nonoscillatory Central Schemes For Multidimensional Hyperbolic Conservation Laws, SIAM Journal on Scientific Computing, 19(6), 1892—1917.

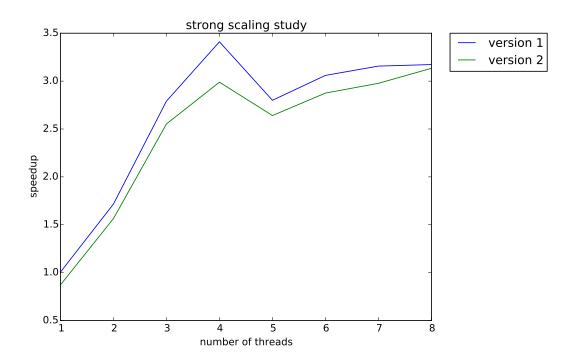


Figure 1: strong scaling

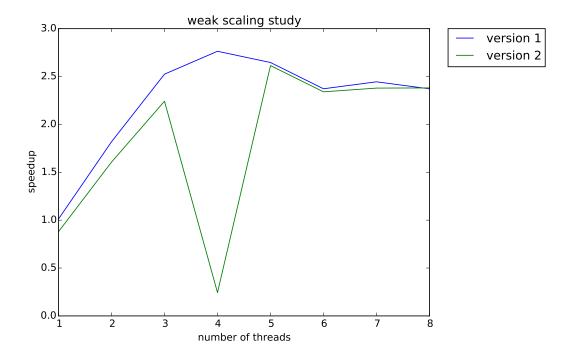


Figure 2: weak scaling

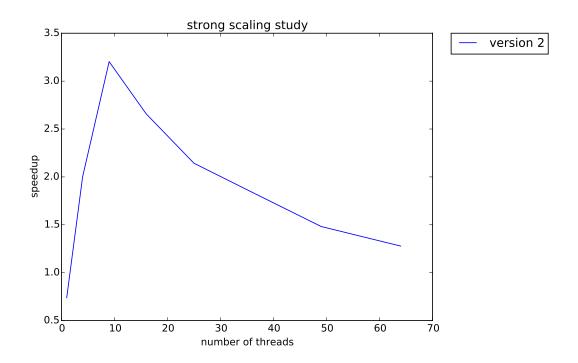


Figure 3: strong scaling

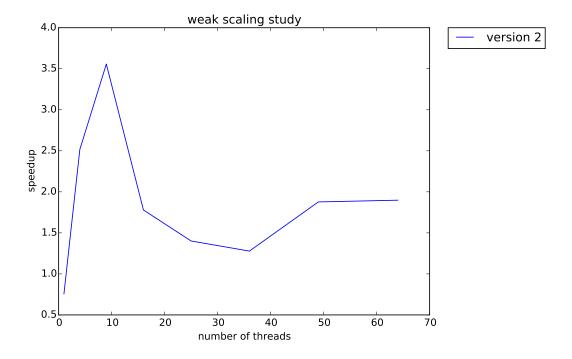


Figure 4: weak scaling

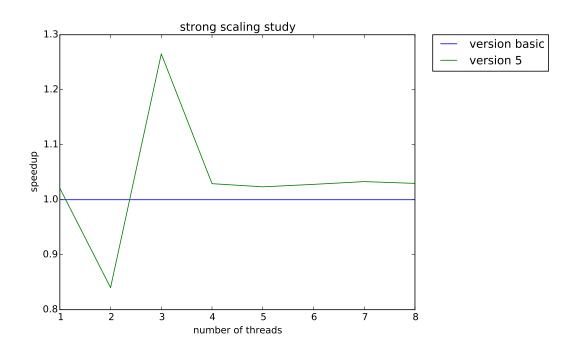


Figure 5: strong scaling

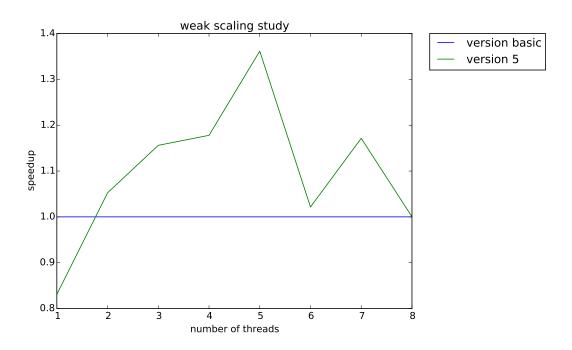


Figure 6: weak scaling

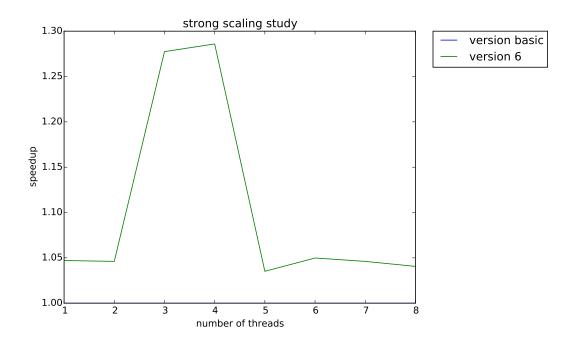


Figure 7: strong scaling

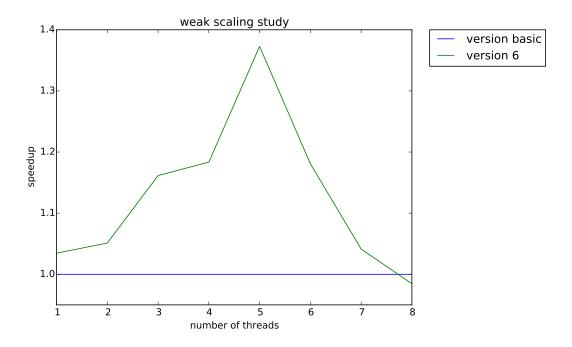


Figure 8: weak scaling

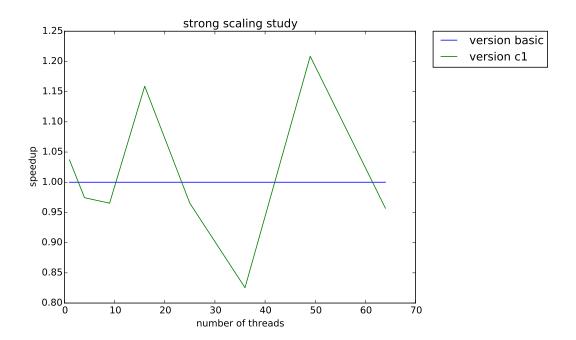


Figure 9: strong scaling

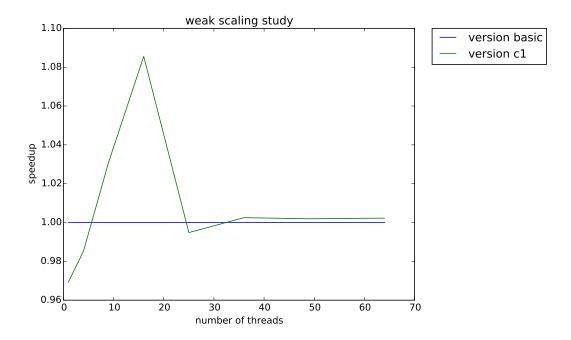


Figure 10: weak scaling

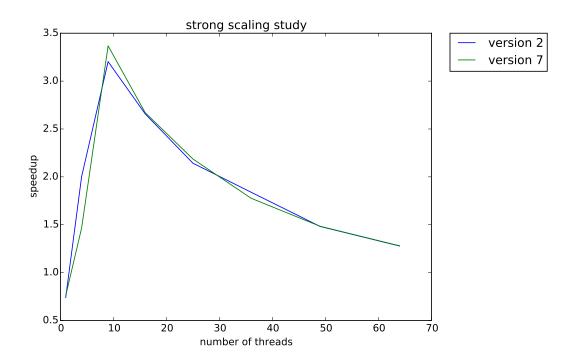


Figure 11: strong scaling

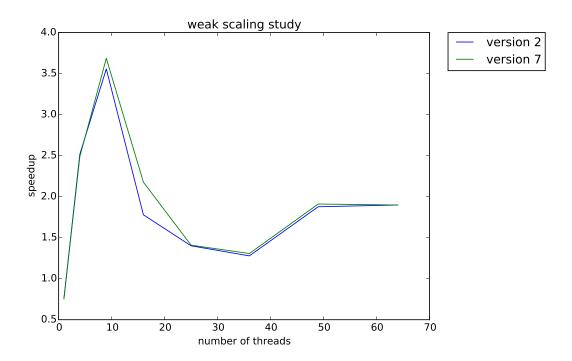


Figure 12: weak scaling

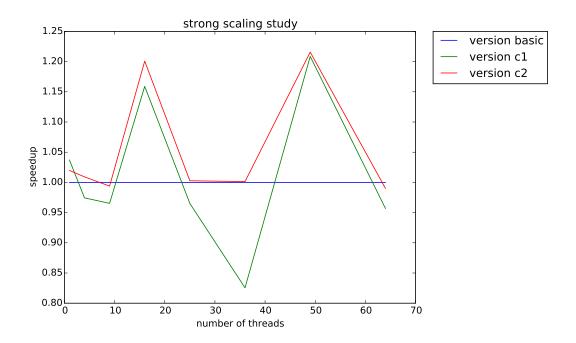


Figure 13: strong scaling

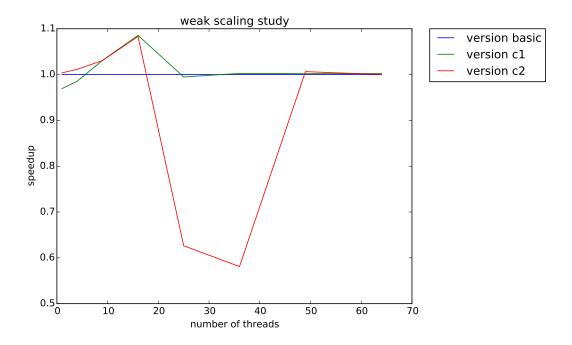


Figure 14: weak scaling

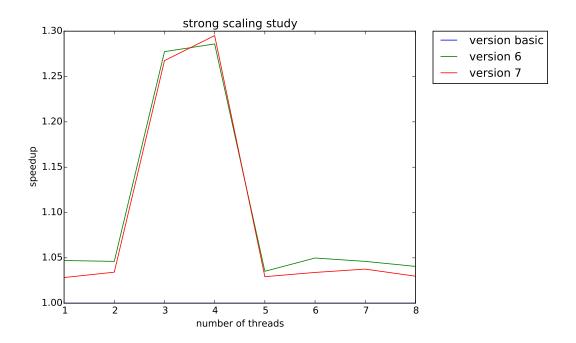


Figure 15: strong scaling

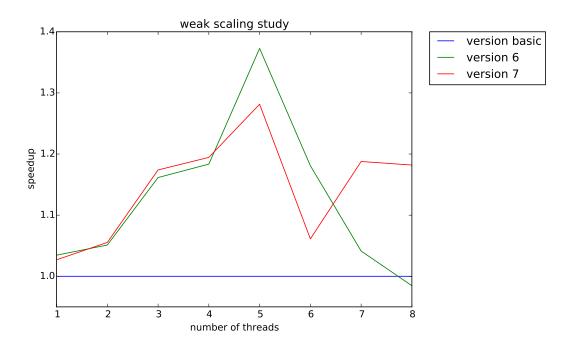


Figure 16: weak scaling