2.3. Vector classes Library

Exercises are located at Exercises/3_Vc/
Solutions are located at Exercises/3_Vc/***/***_solution.cpp
To compile and run exercise programs use the line given in the head-comments in the code.
The results given here are obtained on Intel E7-4860 CPU with gcc4.7.3.

Vc Introduction

Vector classes (Vc) is a free software library to ease explicit vectorization of C++ code. It has an intuitive interface and provides portability between different compilers and compiler versions as well as portability between different vector instruction sets. Thus an application written with Vc can be compiled for AVX, SSE, XeonPhi (MIC) and others SIMD instructions¹.

Similar to the SIMD header files, it provides all basic arithmetic operations and functions, and much more in addition. All functionality, which the headers provide for **fvec** can be used similarly with the class **float v**. The most useful functionalities of Vc are masks and random memory access.

The mask functionality allows conditioning calculations. For example, an absolute value of **a** can be calculated as:

```
float_m mask = (a < 0); a(mask) = -a;
```

Here **mask** saves the comparison result for each entry of **a** in a form, which can be represented like [true;true;false;true] and **operator()** applies the assignment only to those entries, where the mask is true.

The random memory access functionality is provided by the **gather** and **scatter** functions. For example: **gather** fills a vector **a** from an array **A** taking elements with indexes stored in a vector **I**:

a.gather(A, I); // A[I] -> a scatter makes the opposite - fills an array entries from a vector:
a.scatter(A, I); // a -> A[I]

3_Vc/0_Matrix: description

The Matrix exercise requires to parallelize the square root extraction over a set of float variables arranged in a square matrix using the Vc library. The initial code implements scalar and vector parts using the SIMD header, the space for the Vc implementation is blank. Therefore the initial output shows 0 time for vector calculations and infinite speed up factor, that should be currently ignored.

¹ http://code.compeng.uni-frankfurt.de/projects/vc

```
Part of the source code of Matrix.cpp
     float a[N][N] __attribute__ ((aligned(16)));
26
27
     float c[N][N] __attribute__ ((aligned(16)));
     float c_simd[N][N] __attribute__ ((aligned(16)));
28
29
     float c_simdVc[N][N] __attribute__ ((aligned(16)));
30
31
     template<typename T> // required calculations
32
    T f(T x) {
33
       return sqrt(x);
34
...
49
     int main() {
50
51
         // fill classes by random numbers
52
       for( int i = 0; i < N; i++ ) {
53
         for( int j = 0; j < N; j++ ) {
           a[i][j] = float(rand())/float(RAND_MAX); // put a random value, from 0 to
54
     1
55
         }
       }
56
57
58
         /// -- CALCULATE --
59
         /// SCALAR
60
       TStopwatch timerScalar;
61
       for( int ii = 0; ii < NIter; ii++ )</pre>
62
         for( int i = 0; i < N; i++ ) {
63
           for( int j = 0; j < N; j++ ) {
64
             c[i][i] = f(a[i][i]);
65
           }
66
         }
67
       timerScalar.Stop();
68
69
         /// SIMD VECTORS
70
       TStopwatch timerSIMD;
71
       for( int ii = 0; ii < NIter; ii++ )</pre>
72
         for( int i = 0; i < N; i++ ) {
73
           for( int j = 0; j < N; j+=fvecLen ) {
74
               fvec &aVec = (reinterpret cast<fvec&>(a[i][j]));
75
               fvec &cVec = (reinterpret_cast<fvec&>(c_simd[i][j]));
76
               cVec = f(aVec);
77
           }
78
79
       timerSIMD.Stop();
80
81
        /// Vc
82
       TStopwatch timerVc;
83
       //TODO write the code using Vc
84
       timerVc.Stop();
```

```
Typical output

Time scalar: 798.745 ms
Time headers: 201.086 ms, speed up 3.97215
Time Vc: 0 ms, speed up inf
SIMD and scalar results are the same.
ERROR! SIMD and scalar results are not the same.
```

3_Vc/0_Matrix: solution

Since **float_v** is stored in memory in the same way as **fvec** and the function **f(...)** is a template, the part for Vc can be exactly the same, simply the name of the type must be changed:

```
Part of the source code of Matrix solution.cpp
81
         /// Vc
82
       TStopwatch timerVc;
83
       for( int ii = 0; ii < NIter; ii++ )</pre>
84
         for( int i = 0; i < N; i++ ) {
85
           for( int j = 0; j < N; j+=float v::Size ) {</pre>
86
               float v &aVec = (reinterpret cast<float v&>(a[i][i]));
87
               float v &cVec = (reinterpret cast<float v&>(c simd[i][j]));
88
               cVec = f(aVec):
89
           }
90
         }
91
       timerVc.Stop();
     Typical output after solution
     Time scalar: 798.728 ms
     Time headers: 201.078 ms, speed up 3.97223
                   201.079 ms, speed up 3.97221
     SIMD and scalar results are the same.
     SIMD and scalar results are the same.
```

Since 4 float variables fit into a single SIMD vector, all calculations are done in parallel and no overhead operations are required, the expected speed-up factor should be 4.

3_Vc/1_QuadraticEquation: description

The QuadraticEquation exercise requires to vectorize using Vc the solution of a set of quadratic equations in three different ways, based on tree different data setups: (1) Array of Structures (AoS), (2) Structure of Arrays (SoA) (3) Array of Structures of Arrays (AoSoA).

It is recommended to compile the code with **-fno-tree-vectorize** option to prevent auto-vectorization of the scalar code, otherwise the comparison of the vectorized and scalar codes will not be direct.

The input data is given already in the required formats. An elemental structure **DataAOSElement**, which contains parameters of the equations and the resulting maximum root, is declared for the AoS format. **_mm_malloc** function is used to allocate aligned memory.

```
Part of the source code of QuadraticEquation.cpp
23
     struct DataAOSElement {
24
       float a, b, c, // coefficients
25
         x; // a root
26
    };
27
28
     struct DataAOS {
29
       DataAOS(const int N) {
30
         data = (DataAOSElement*) _mm_malloc(sizeof(DataAOSElement)*N,16);
31
32
       ~DataAOS() {
33
         if(data) _mm_free(data);
34
35
       DataAOSElement *data;
36
    };
```

The SoA format is declared as a whole structure, which contains dynamic arrays.

```
Part of the source code of QuadraticEquation.cpp
     struct DataSOA {
38
39
40
       DataSOA(const int N) {
41
         a = (float*) _mm_malloc(sizeof(float)*N,16);
42
         b = (float*) _mm_malloc(sizeof(float)*N,16);
43
         c = (float*) _mm_malloc(sizeof(float)*N,16);
44
         x = (float*) mm malloc(sizeof(float)*N,16);
45
       }
46
      ~DataSOA()
47
48
         if(a) _mm_free(a);
49
         if(b) _mm_free(b);
50
         if(c) _mm_free(c);
51
         if(x) mm free(x);
52
       }
53
54
       float *a, *b, *c, // coefficients
55
         *x; // a root
56
     };
```

To define the AoSoA format an elemental structure **DataAOSOAElement** is declared to contain information about **float_v::Size** (4) equations, similarly to **DataSOA**. The elemental structures are packed together in the DataAOSOA structure similarly to **DataAOS**. Memory for all information is allocated in one go in **DataAOSOA** to ensure compact data allocation, afterwards the memory is distributed between elemental structures using **SetMemory** function.

```
Part of the source code of QuadraticEquation.cpp
58
     struct DataAOSOAElement {
59
60
       void SetMemory(float *m) {
61
         a = m;
62
         b = m + float_v::Size;
63
         c = m + 2*float_v::Size;
64
         x = m + 3*float_v::Size;
65
66
67
       float *a, *b, *c, // coefficients
68
         *x; // a root
69
    };
70
71
     struct DataAOSOA {
72
       DataAOSOA(const int N) {
73
         const int NVectors = N/float_v::Size;
74
75
         data = new DataAOSOAElement[NVectors];
76
         memory = (float*) _mm_malloc(sizeof(float)*4*N,16);
77
78
         float *memp = memory;
79
         for( int i = 0; i < NVectors; i++ ) {</pre>
80
           data[i].SetMemory(memp);
81
           memp += float_v::Size*4;
82
         }
83
       }
84
      ~DataAOSOA() {
85
         _mm_free(memory);
86
         delete[] data;
87
       }
88
89
       float *memory;
90
       DataAOSOAElement *data;
91
```

The given structures is filled by the same random data sample and scalar implementation is given in the exercise code.

```
Part of the source code of QuadraticEquation.cpp
150
       // fill parameters by random numbers
151
       for( int i = 0; i < N; i++ ) {
         float a = 0.01 + float(rand())/float(RAND_MAX); // put a random value, from
152
     0.01 to 1.01 (a has not to be equal 0)
153
         float b = float(rand())/float(RAND_MAX);
154
         float c = -float(rand())/float(RAND_MAX);
155
156
         dataScalar.data[i].a = a;
157
         dataScalar.data[i].b = b;
158
         dataScalar.data[i].c = c;
159
160
         dataSIMD1.data[i].a = a;
161
         dataSIMD1.data[i].b = b;
162
         dataSIMD1.data[i].c = c;
163
164
         dataSIMD2.a[i] = a;
165
         dataSIMD2.b[i] = b;
166
         dataSIMD2.c[i] = c;
167
168
         const int nV = i/float v::Size;
169
         const int iV = i%float v::Size;
170
         dataSIMD3.data[nV].a[iV] = a;
171
         dataSIMD3.data[nV].b[iV] = b;
172
         dataSIMD3.data[nV].c[iV] = c;
173
       }
174
175
       /// -- CALCULATE --
176
177
       // scalar calculations
178
       TStopwatch timerScalar;
179
       for(int io=0; io<NIterOut; io++)</pre>
180
         for(int i=0; i<N; i++)</pre>
181
182
           float &a = dataScalar.data[i].a:
183
           float &b = dataScalar.data[i].b;
184
           float &c = dataScalar.data[i].c;
185
           float &x = dataScalar.data[i].x;
186
187
           float det = b*b - 4*a*c;
188
           x = (-b+sqrt(det))/(2*a);
189
         }
190
       timerScalar.Stop();
     Typical output
     Time scalar:
                    567.055 ms
     Time Vc AOS:
                    0 ms, speed up inf
                    0 ms, speed up inf
     Time Vc SOA:
    Time Vc AOSOA: 0 ms, speed up inf
     ERROR! SIMD and scalar results are not the same. SIMD part 1.
     ERROR! SIMD and scalar results are not the same. SIMD part 2.
     ERROR! SIMD and scalar results are not the same. SIMD part 3.
```

3_Vc/1_QuadraticEquation: solution

(1) To vectorize the AoS format one needs to gather data from different instances of the **DataAOSElement** structure and pack it together (in groups by 4) in **float_v** variables. Since the same data (for example, the **a** variable) is placed in different parts of memory, data coping is necessary here. Ones data is grouped, the solution is found using exactly the same code as one given in the scalar part. The data is ungrouped back into the output **x** variable.

```
Part of the source code of QuadraticEquation solution.cpp
194
       for(int io=0; io<NIterOut; io++)</pre>
195
196
         for(int i=0; i<NVectors; i++)</pre>
197
198
           // copy input data
199
           float_v aV;
200
           float_v bV;
201
           float_v cV;
202
203
204
           for(int iV=0; iV<float v::Size; iV++)</pre>
205
206
             aV[iV] = dataSIMD1.data[i*float v::Size + iV].a;
207
             bV[iV] = dataSIMD1.data[i*float v::Size + iV].b;
208
             cV[iV] = dataSIMD1.data[i*float_v::Size + iV].c;
209
           }
210
211
           const float_v det = bV*bV - 4*aV*cV;
212
           float v xV = (-bV+sqrt(det))/(2*aV);
213
214
           // copy output data
215
           for(int iE=0; iE<float_v::Size; iE++)</pre>
216
             dataSIMD1.data[i*float v::Size+iE].x = xV[iE];
217
         }
218
       }
```

(2) The second task is vectorization with the SoA data format. Since in SoA similar data is placed near each other, the **reinterpret_cast** can be used. Ones the data is reinterpreted, the solution is found using exactly the same code, as the given one in the scalar part.

```
Part of the source code of QuadraticEquation solution.cpp
223
       for(int io=0; io<NIterOut; io++)</pre>
224
         for(int i=0; i<N; i+=float_v::Size)</pre>
225
226
           float_v& aV = (reinterpret_cast<float_v&>(dataSIMD2.a[i]));
227
           float v& bV = (reinterpret cast<float v&>(dataSIMD2.b[i]));
228
           float_v& cV = (reinterpret_cast<float_v&>(dataSIMD2.c[i]));
229
           float_v& xV = (reinterpret_cast<float_v&>(dataSIMD2.x[i]));
230
231
           const float_v det = bV*bV - 4*aV*cV;
232
           xV = (-bV + sqrt(det))/(2*aV);
233
         }
```

(3) The third task is vectorization with the AoSoA data format. The reinterpret cast can be used here in the same way as with the SoA format, just the dereference operator must be applied in addition. The calculations part remains the same as well.

```
Part of the source code of QuadraticEquation solution.cpp
238
       for(int io=0; io<NIterOut; io++)</pre>
239
         for(int i=0; i<NVectors; i++)</pre>
240
241
           float_v& aV = *(reinterpret_cast<float_v*>(dataSIMD3.data[i].a));
242
           float_v& bV = *(reinterpret_cast<float_v*>(dataSIMD3.data[i].b));
243
           float v& cV = *(reinterpret cast<float v*>(dataSIMD3.data[i].c));
244
           float v& xV = *(reinterpret cast<float v*>(dataSIMD3.data[i].x));
245
246
           const float_v det = bV*bV - 4*aV*cV;
247
           xV = (-bV + sqrt(det))/(2*aV);
248
```

```
Typical output after solution

Time scalar: 566.821 ms
Time Vc AOS: 217.513 ms, speed up 2.60592
Time Vc SOA: 142.603 ms, speed up 3.97482
Time Vc AOSOA: 143.57 ms, speed up 3.94805
SIMD 1 and scalar results are the same.
SIMD 2 and scalar results are the same.
SIMD 3 and scalar results are the same.
```

The speed up factor of 4 is expected due to vectorization. It is achieved with the SoA and AoSoA data formats. With AoS additional data regrouping is required, that results in the smaller speed up of 2.6.

3_Vc/2_Newton: description

The Newton exercise requires to vectorize the Newton method for numerical solution of a group of equations.

The method can be explained graphically as in the Fig 1. The task is to find intersection of the curve and the X-axis. The algorithm starts with an initial approximation for root x_0 and takes a function value at

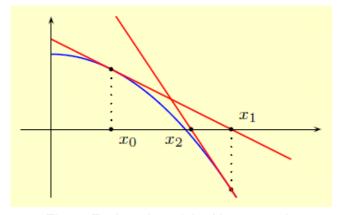


Fig. 1. Explanation of the Newton task.

this point. A tangent line is drown at this point, an intersection of the tangent line with the X-axis is the next approximation x_1 :

```
x_k \equiv x_{k-1} - f(x_{k-1})/f'(x_{k-1})
```

Then the procedure is repeated until the approximation does not change within the required precision.

```
x_k - x_{k-1} < epsilon
```

A scalar version of the algorithm is given in the exercise. A solution is proposed to perform in two steps. First, vectorize the algorithm, which uses a fixed number of iterations (1000). Then make the number of iterations dependent on the required precision. The vectorized version must give exactly the same result as the scalar one.

```
Part of the source code of Newton.cpp
44
     float FindRootScalar(const float& p1, const float& p2)
45
46
       float x = 1, x new = 0;
47
       for(; abs((x_new - x)/x_new) > P; ) {
48
           // for(int i = 0; i < 1000; ++i){
49
         x = x_new;
50
         x_{new} = x - F(x,p1,p2) / Fd(x,p1,p2);
51
52
       return x_new;
    Typical output
     Scalar part:
    Results are correct!
    Time: 15.415 ms
    SIMD part:
    Results are NOT the same!
    Time: 0.226021 ms
     Speed up: 68.2015
```

3_Vc/2_Newton: solution

The parallelization is achieved by grouping 4 equations together. A complication in this case is that different equations will reach the required precision at different number of iterations. This problem can be solved using Vc masks: the loop exit condition should be stored as a mask. Then the loop is continued until the mask has at least one entry with the value **true**. A mask value should be also used during update of the root approximation in order to reproduce the scalar result.

```
Part of the source code of Newton solution.cpp
56
     float v FindRootVector(const float v& p1, const float v& p2)
57
     {
58
       float_v x = 1.f, x_new = 0.f;
59
       float_m mask(true);
60
       for( ; !mask.isEmpty(); ) {
61
           // for(int i = 0; i < 1000; ++i){
62
         x = x \text{ new};
63
         x_{new}(mask) = x - F(x,p1,p2) / Fd(x,p1,p2);
64
         mask = abs((x_new - x)/x_new) > P;
65
66
       return x_new;
67
     Typical output after solution
     Scalar part:
    Results are correct!
     Time: 15.3401 ms
     SIMD part:
     Results are the same!
     Time: 4.49395 ms
     Speed up: 3.4135
```

A typical speed up factor of vectorization is 4, but since mask is used, the parallelization is not full and at the final iterations only a part of the SIMD vector entries is used. Therefore, the speed up factor is about 3.5.

3_Vc/3_RandomAccess: description

The RandomAccess exercise requires to use different forms of the **gather** and **scatter** functions. For that an input array of **float** is provided and randomly filled. Also an array of random indices is provided. It is required to (1) gather data from the **input** array to the tmp **float_v** variable according to the **index** array; (2) similarly, gather the data, but only when it satisfies a given condition; (3) put the data from the tmp **float_v** variable to the **output** array, when it satisfies a given condition.

```
Part of the source code of RandomAccess.cpp
21
     float input[N];
22
     float output[N];
23
24
     int main() {
25
26
       unsigned int index[float_v::Size];
27
30
       // fill input array with random numbers from 0 to 1
31
       for( int i = 0; i < N; i++ ) {
32
         input[i] = float(rand())/float(RAND_MAX);
33
       }
34
35
       // fill output array with 0
36
       for( int i = 0; i < N; i++ ) {
37
         output[i] = 0;
38
       }
39
40
       // fill indices with random numbers from 0 to N-1
41
       for( int i = 0; i < float_v::Size; i++) {</pre>
42
         index[i] = static_cast<unsigned int>(float(rand())/float(RAND_MAX)*N);
43
       }
44
45
       cout << "Indices: ";</pre>
46
       for(int i=0; i<float_v::Size; i++)</pre>
47
         cout << index[i] << " ";</pre>
48
       cout << endl;
49
50
         /// gather without masking
51
       float_v tmp;
52
       //TODO gather data with indices "index" from the array "input" into float_v
53
       // Use void gather (const float *array, const uint v &indexes)
65
         /// gather with masking
66
       float_v tmp2;
       //TODO gather data with indices "index" from the array "input" into float v
67
     tmp2, if the value of "input" large then 0.5
       // Use void gather (const float *array, const uint_v &indexes, const float_m
68
     &mask)
       //TODO create mask for values for an obtained tmp values, which are large
91
     than 0.5 and
       //TODO put all values smaller than 0.5 from tmp to the array "output" at the
92
     places given by indices "index"
       // Use void scatter (float *array, const uint v &indexes, const float m
93
     &mask) const
```

```
Typical output

Indices: 25 96 76 42
Gather without masking: results are WRONG.
-4.67253e+33 is not equal to 0.988475
4.59163e-41 is not equal to 0.912037
0 is not equal to 0.80679
Gather with masking: results are WRONG.
Scatter with masking: results are correct.
```

3_Vc/3_RandomAccess: solution

(1) To gather data from the given places in an array, one needs to create a **uint_v** vector with corresponding indexes, then the **gather** function can be applied directly.

```
Part of the source code of RandomAccess_solution.cpp

53    uint_v ind(index);
54    tmp.gather(input,ind);
```

(2) To gather data under the given condition, one needs to create a mask with a corresponding type. Since the data is **float**, the **float_m** mask must be created, then the **gather** function with the mask parameter is applied directly. To ensure that the entries, which were masked out, have meaningful values, we need to initialise the output variable before gathering.

```
Part of the source code of RandomAccess_solution.cpp

float_m mask = tmp > 0.5f;
float_v tmp2(Vc::Zero);
tmp2.gather(input, ind, mask);
```

(3) To scatter data under the given condition one needs to create a mask with a corresponding type. Since the data is **float**, the same mask can be used as in (2), then the **scatter** function with the mask parameter is applied directly.