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Set 2 - SIMD and BLAS

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Question 1: SIMD force calculation

```
1  /// compute the Lennard-Jones force acting on one particle at position x0
2  scalar_type compute_force(std::vector<scalar_type> const& positions,
3                            scalar_type x0, scalar_type rc)
4  {
5      scalar_type rm2 = rm * rm;
6      scalar_type force = 0.;
7      for (size_type i=0; i<N; ++i) {
8          if (std::abs(r) < rc) {
9              scalar_type r2 = r * r;
10             scalar_type s2 = rm2 / r2;  // (rm/r)^2
11             scalar_type s6 = s2*s2*s2;  // (rm/r)^6
12             force += 12*eps * (s6*s6 - s6) / r;
13         }
14     }
15     return force;
16 }
```

Listing 1: `calculate_force` function included in `force1d.cpp`

The code above is a simple force calculation for a one-dimensional nbody problem. In this exercise you should have to speedup the `calculate_force` with manual SIMD.

a) Implement the loop with manual SSE intrinsics (or AVX if you have a suitable machine). As you cannot branch depending on the value of `r` when processing several values with one instruction, you need to avoid any `if` statements.

   Hint: The comparison intrinsics like `_mm_cmplt_ps` create a mask depending on the outcome of the comparison. In a logic operation like `_mm_and_ps` this mask can be used to set all vector elements to zero for which the comparison yielded `false`.

b) Discuss how the force calculation of the attached two-dimensional Molecular Dynamics code can be vectorized. Is a different data layout for the particle positions more suited to SIMD vectorization? Sketch how the periodic boundaries can be implemented with SIMD intrinsics, i.e. without branching.

Question 2: BLAS

In this exercise you should familiarize yourself with general matrix multiplications (GEMM) using a BLAS library. We provide you with a skeleton code where you should replace the matrix multiplication with a call to GEMM. Finish the skeleton code and install a BLAS library on your personal system.

a) Report on what version of BLAS you are using, how you can link to it, if it is single-threaded or multi-threaded, and how can you specify the number of threads in the multi-threaded version. How much faster is your code with BLAS compared to the trivial implementation of the matrix multiplication in the skeleton code?

b) Same as a) except that the code has to run on EULER.

Summary

Summarize your answers, results and plots into a PDF document. Furthermore, elucidate the main structure of the code and report possible code details that are relevant in terms of accuracy or performance. Send the PDF document and source code to your assigned teaching assistant.