

# Preface

## Overview and Goals

Molecular dynamics simulation (MD) as such has long matured and has become a valuable tool in a variety of disciplines. For several reasons, however, MD is just about to evolve as a general tool in engineering sciences. In process engineering in particular, the development of MD simulation has become a focus of research during the last years and still gains momentum, slowly undergoing the transition from a scholarly academic occupation to a key technology in industrial-scale fluid process engineering. Central to ongoing efforts in Germany is the development of the simulation code `ls1 mardyn`, which has now been developed for over a decade in an interdisciplinary cooperation of researchers in process engineering high-performance computing (HPC).

It is the purpose of this book to present modern implementations of relevant MD algorithms at the example of `ls1 mardyn`, a simulation code targeting engineering applications. Thereby, we strictly focus on HPC-related aspects. We cover the implementation on HPC architectures, taking Intel Xeon and Intel Xeon Phi clusters as representatives of current platforms. We describe the distributed- and shared-memory parallelization, including load balancing, on these platforms and particularly focus on the efficient implementation of the compute kernels. Thereby, we also describe the software-architecture of the resulting code.

The developments presented here approximately cover work of the years 2008–2014, and have been spread over (at least) three dissertations and several publications. Motivated by the positive perception of our work in the community and the recognition of our work at the International Supercomputing Conference 2013 (ISC'13) with the PRACE ISC Award, we aim to give a comprehensive and unified description of our efforts.

## Organization of the Book

In this work, we place the emphasis on the efficient implementation and parallelization of a MD code. In order to build a solid basis to understand the important characteristics of such a simulation code, we cover modeling approaches as far as they are relevant to process engineering, and give a concise description of the basic MD algorithms. Based on that description, we motivate the development of a simulation code specialized on process engineering applications, and discuss the software structure of the code `ls1 mardyn`. To understand the requirements on an efficient implementation of the relevant algorithms on current hardware, we give a rather deep explanation of the Intel Xeon and Intel Xeon Phi. Subsequently, we detail the parallel implementation of MD simulation on these systems making use of shared- and distributed-memory parallelization, including an efficient load-balancing scheme. Most focus is put on the efficient vectorization of the compute kernels for the target processors, using intrinsics. The described implementations are extensively benchmarked through runtime experiments. In addition to the optimized production version of the simulation code `ls1 mardyn`, a hybrid parallel version simultaneously making use of the Intel Xeon Phi co-processor and the Intel Xeon-based host system is evaluated, as well as a version specialized on atomic fluids, which is executed on up to 146,016 cores on the SuperMUC cluster.

## Target Audience

This contribution mainly targets readers at the postgraduate and Ph.D. level in the broad field of scientific computing—where MD simulation, process engineering, computer science, and HPC coalesce. We believe that the presented research can serve both as a good starting point for further research as well as a source of ideas about alternative approaches.

## Acknowledgments

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