The prevalence of multi-core CPUs during the last decade has provided scientists with the possibility of conducting large-scale computer simulations. However, the multi-core architecture brought not only improved computing capabilities but also more programming challenges due to more complex memory hierarchies.

In this thesis, we study how to efficiently utilize the computing power of multi-core CPUs and how to analyze the code performance obtainable on this hardware architecture. A series of interdisciplinary real-world scientific applications have been selected as the cases of study, which arise from computational cardiology and computational geoscience.

The PhD investigation has been carried out from different angles: numerical algorithms, parallel programming and performance modeling and prediction. For two applications of cardiology, mixed programming and relevant optimization strategies have produced good performance for multi-core based clusters, when the solution domain is irregular. In three other geoscience applications, we have studied how to use compressed data structures, optimize cache usage and effectively parallelize various numerical schemes for the multi-core architecture. A practical approach to analyzing and predicting code performance is also proposed.

It is shown that code implementation and optimization must match both the involved computations and the target parallel platform. Several good practices are summarized for parallel programming and performance analysis on the multi-core architecture, which can be of help to many other scientists.