Automated optimisation of quantum chemical algorithms within an integrated tensor framework

Christoph Köppl[1], Gerald Knizia[1] and Hans-Joachim Werner[1]

[1] Institut für Theoretische Chemie, Universität Stuttgart, Germany

The manual implementation of quantum chemical ab initio methods can become unpractical and error-prone once a certain degree of complexity is exceeded. Therefore, automation tools that help simplifying method implementation processes are increasingly important.

Along these lines, we present a tool to optimise high-level algorithms towards memory and I/O efficiency in the context of the Integrated Tensor Framework (ITF) [1, 2] developed by G. Knizia. In this tensor framework, algorithms are composed of abstract high-level instructions, e.g. to access tensors, create loops or to perform tensor contractions, and these algorithms are executed on a virtual machine (VM) within the ITF at runtime.

In order to assemble memory and I/O efficient algorithms for complex methods consisting of many interconnected binary contractions, the optimisation tool makes particularly use of the following algorithmic manipulations: (1) the introduction of loops, (2) the reuse of tensors and (3) the optimisation of the contraction order. Starting from sets of coupled binary tensor contractions and corresponding tensor properties, a combination of dedicated heuristics and Simulated Annealing is then used for optimisations in the present large optimisation space. This optimisation strategy can be applied to a large range of methods within the ITF; including CCSD, CCSD gradients, DF-CASPT2 gradients [3] and MRCIC [1].

Selected benchmark examples furthermore present the usefulness of this optimisation approach for various ab initio methods available within the ITF.

[1] K. R. Shamasundar, Gerald Knizia, and Hans-Joachim Werner, *The Journal of Chemical Physics*, 135(5):054101, 2011.

[2] Hans-Joachim Werner, Peter J. Knowles, Gerald Knizia, Frederick R. Manby, and Martin Schütz, *Wiley Interdisciplinary Reviews: Computational Molecular Science*, 2(2):242, 2012.

[3] Werner Győrffy, Toru Shiozaki, Gerald Knizia and Hans-Joachim Werner *The Journal of Chemical Physics*, 138(10):104104, 2013