Dense linear algebra software stack

BLAS-like Library Instantiation Software (BLIS). This portable framework for rapidly instantiating BLAS-like libraries is a refactoring of Kazushige Goto’s approach to the implementation of the level-3 BLAS. Importantly, BLIS offers virtually all level-3 computation in terms of a single “micro-kernel,” and thus serves as a productivity lever when supporting existing BLAS and custom BLAS-like matrix operations. BLIS also exposes new opportunities for optimization and parallelization, both within the framework itself as well as higher-level DLA implementations typically found in LAPACK. Level-2 operations were also restructured, exposing key so-called level-1 (vector) and level-1 (fused) kernel operations.

Application in Computation Chemistry

Coupling a Modern DLA Stack to a Modern Computational Chemistry (Coupled Cluster) Stack

We are working on coupling the BLIS framework more tightly with the recently-developed NCC module in the CFOUR program suite. This module is a modern C++ software stack for performing Coupled Cluster (CC) and CC-like calculations. NCC has recently been applied to a variety of applications in quantum chemistry. CC calculations may significantly benefit by exposing pieces of the linear algebra stack beyond the traditional BLAS interface.

Recent publications

- T. M. Low, F. D. Igual, T. M. Smith, and E. S. Quintana-Orti. Analytical Modeling is Enough for High-Performance BLAS. ACM TOMS (pending modifications).

Training the next generation of computational scientists

Software developed by this project is being distributed by AMD, ARM, Texas Instruments, and Movidius. It is also at the core of research collaborations with Intel and HP.

Recent publications

- Communication: The performance of non-iterative coupled cluster quadruples models.
- CCSDT-GF calculations of molecular thermochemistry and kinetics.
- High-accuracy thermochemistry and kinetics.
- Communication: The performance of non-iterative coupled cluster quadruples models.
- Communication: The performance of non-iterative coupled cluster quadruples models.