

NUMERICAL ANALYSIS AND SCIENTIFIC COMPUTING  
SEMINAR

*Techniques for High-Performance Construction of Fock  
Matrices*

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**Abstract:** This work presents techniques for high performance Fock matrix construction when using Gaussian basis sets. Three main techniques are considered. (1) To calculate electron repulsion integrals, we demonstrate batching together the calculation of multiple shell quartets of the same angular momentum class so that the calculation of large sets of primitive integrals can be efficiently vectorized. (2) For multithreaded summation of entries into the Fock matrix, we investigate using a combination of atomic operations and thread-local copies of the Fock matrix. (3) For distributed memory parallel computers, we present a globally-accessible matrix class for accessing distributed Fock and density matrices. The new matrix class introduces a batched mode for remote memory access that can reduce synchronization cost. The techniques are implemented in an open-source software library called GTFock.

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