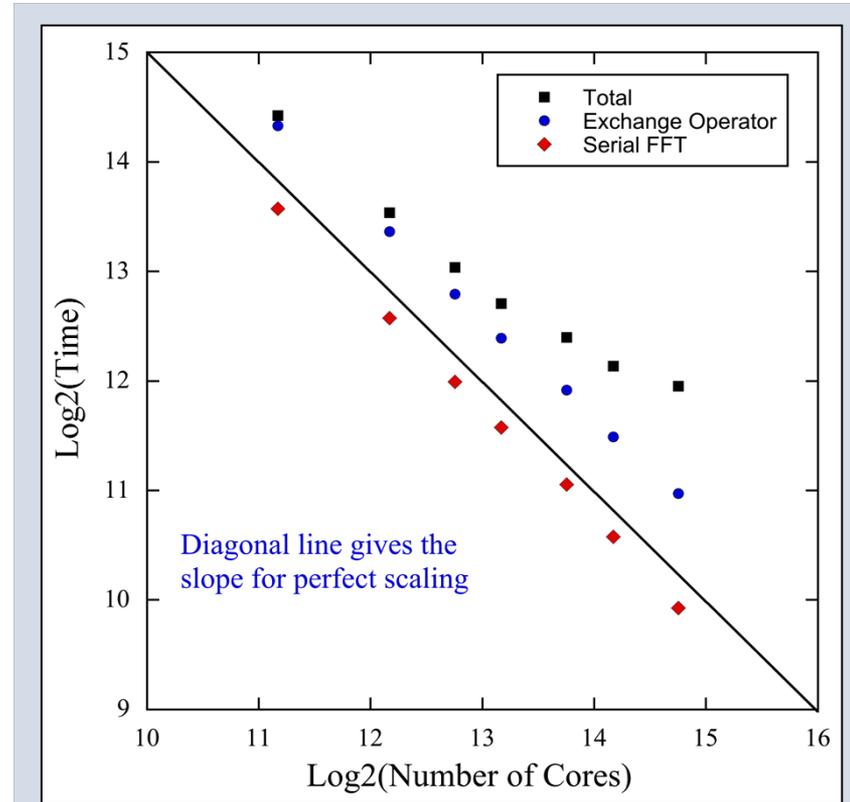


A new algorithm for constructing the exchange operator in density-functional-theory calculations using hybrid functionals

SAND# 2015-

- Scaling tests of the new algorithm were performed for a mission relevant 256-atom supercell of bulk gold using density-functional theory (DFT) and the Heyd-Scuseria-Ernzerhof (HSE) hybrid functional implemented in the (SNL) Socorro code.
- Runs using 2304 ($2^{11.1699}$) to 27648 ($2^{14.7549}$) exhibited nearly perfect scaling for the construction of the HSE exchange operator, which dominates the total time for in smallest run considered herein and takes about half the total time in the largest run
- The improved scaling of the new algorithm, compared with current algorithms, will enable higher fidelity hybrid DFT calculations for High-Energy-Density-Science and Radiation Effects mission areas at Sandia



Timings for a self-consistent HSE calculation of bulk gold in a 256-atom supercell, demonstrating nearly perfect scaling for the construction of the exchange operator and its serial fast-Fourier transforms (FFT's).

Principal Investigator: Alan F. Wright
 Platform and Campaign ID: Cielo/CCC-8
 Usage: 0.82 days