Development of Buffer Method in Parallelized Molecular Orbital Calculation

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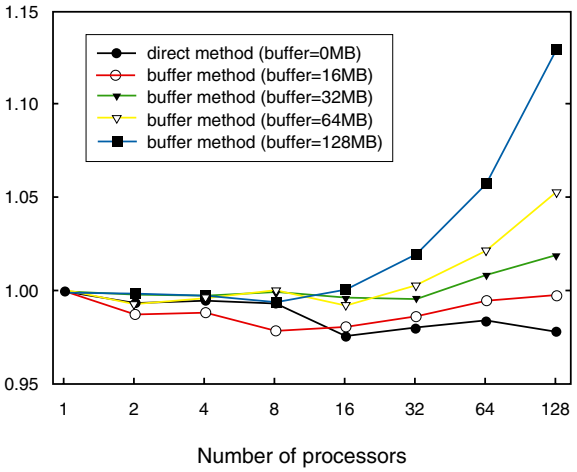
The modified direct SCF-MO method (buffer method) was developed to improve the parallelization efficiency in Fock matrix generation by using a PC cluster that does not have secondary storage on each processor. In this method, in the first SCF cycle, part of the electron repulsion integrals is stored in a buffer (unused memory) and the stored integrals are reused in subsequent SCF cycles. This simple method achieved super-linear scalability.



Parallelization efficiencies of buffer method with various buffer sizes
*Test data: target molecule was Crambin (46 amino-acid residues, 642 atoms), basis set was STO-3G (1974 basis functions)

World's Fastest Fiber-Optic Quantum Key Distribution at 1550 nm

- Toward practical use of quantum cryptographic technology for ultimate security -

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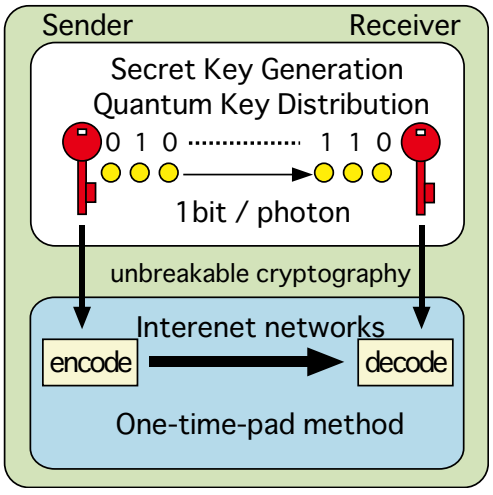
The Photonics Research Institute (PRI) of the National Institute of Advanced Industrial Science and Technology (AIST), one of independent administrative institutions, has developed a thermoelectrically cooled single-photon detector boasting of its fastest operational speed in the world in the wavelength band for optical fiber communication, 1550 nm, based on the AIST-developed epoch-making single-photon detecting technique, discharge pulse counting, and succeeded in demonstrating the world's fastest quantum key distribution at 1550 nm. The repetition rate of single-photon detection was 10 MHz. The key rate was 45 kbit/s when using a 10.5 km long optical fiber as a quantum channel.



Topology of unbreakable cryptography