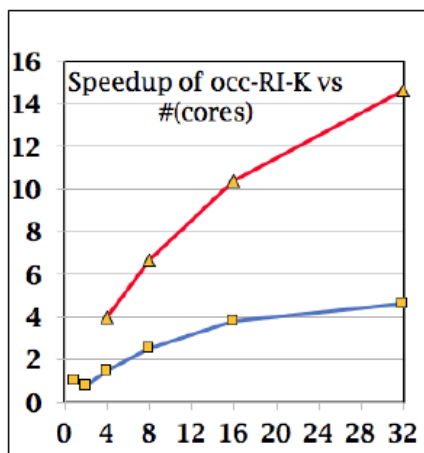
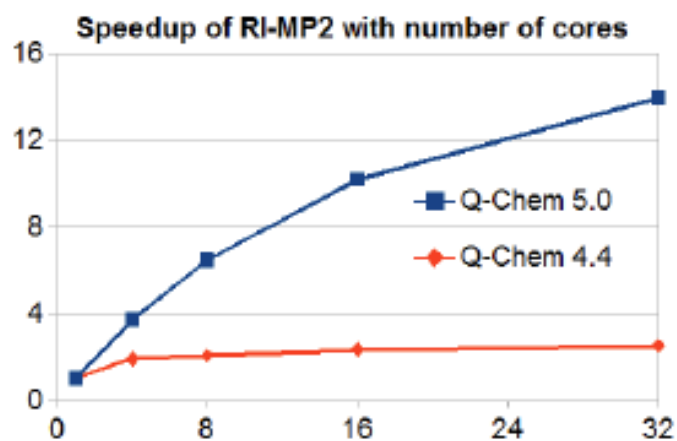


Computational Efficiency



(a) Parallel scaling for Diamond-doid_octahedral (148 atoms, red line) and Vitamin E (81 atoms, blue line)



(b) Parallel scaling for vitamin E molecule (cc-pVDZ, 81 atoms, 684 basis functions)

- **Resolution-of-the-Identity Algorithms for SCF and Post-SCF Calculations:**

- occ-RI-K algorithm for Hartree-Fock exchange;
- RI-SCF gradient;
- I-MP2, SCS-MP2, SOSMP2 methods;
- RI-CCSD and RI-EOM energies and gradients.

- **Fast Algorithms for DFT Calculations:**

- Algorithms for Coulomb (Continuous Fast Multipole Method, J engine, Fourier Transform Coulomb, Quantum Ewald Mesh);
- Algorithms for Hartree-Fock exchange (Link, ARIK) and numerical integration (mrXC).

- **Fast Algorithms for Perturbation Theory Calculations:**

- Fast integral transformations, RI approximation, scaling of different spin components, Laplace transform, dual basis extrapolation, and the use of localized orbitals.

- **Fast Algorithms for Coupled-Cluster Calculations:**

- Enhanced by a modern tensor library, RI approximation, Cholesky decomposition, single-precision execution, frozen natural orbitals.

- **Efficient Implementation on Shared-Memory Multicore Machines; GPU acceleration via BrianQC module; Cloud-Enabled.**

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