ParaGauss

A Program Package for High-Performance Computations of Molecular Systems

ParaGauss is a parallel DFT code for solving challenging electronic structure problems in chemistry, surface science, and the field of nanostructured materials. It is written in the FORTRAN 95 language and parallelized via MPI.

Among other features ParaGauss provides:

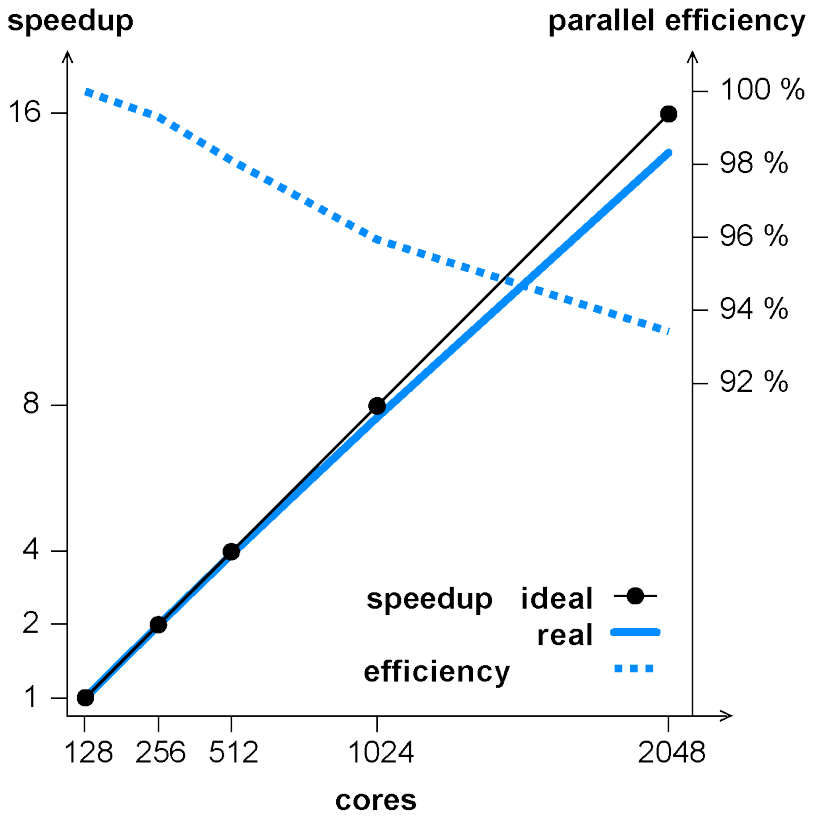
- Calculation of DFT energy and forces
- Local, GGA, meta-GGA, and hybrid exchange-correlation functionals
- Geometry optimization and local search of transition state
- Pseudopotentials as an atomic core substitute
- Relativistic methods for heavy elements including treatment of spin-orbit interaction
- Solvation models
- Environmental models

Contributors

ParaGauss was developed at Technische Universität München by Thomas Belling, Thomas Grauschopf, Sven Krüger, Folke Nörtemann, Markus Staufer, Markus Mayer, Vladimir A. Nasluzov, Uwe Birkenheuer, Aguang Hu, Alexei Matveev, Aleksey V. Shor, Monika Fuchs-Rohr, Konstantin M. Neyman, Dimitry I. Ganyushin, Teerakiat Kerdcharoen, André Woiterski, Sonjoy Majumder, Miquel H. i Rotllant, Raghunathan Ramakrishnan, Gopal Dixit, Astrid Nikodem, Thomas M. Soini, Martin Roderus, and Notker Rösch.

Parallel Performance

Speed-up and efficiency for the example of SCF cycles of the cluster $Pt_{140}(CO)_8$ as calculated with the TPSSh functional together with small core pseudopotentials.



Further Reading

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