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Introducing PROFESS 2.0: A parallelized, fully linear scaling program for orbital-free density functional theory calculations [☆]

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ABSTRACT

Orbital-free density functional theory (OFDFT) is a first principles quantum mechanics method to find the ground-state energy of a system by variationally minimizing with respect to the electron density. No orbitals are used in the evaluation of the kinetic energy (unlike Kohn–Sham DFT), and the method scales nearly linearly with the size of the system. The Princeton Orbital-Free Electronic Structure Software (PROFESS) uses OFDFT to model materials from the atomic scale to the mesoscale. This new version of PROFESS allows the study of larger systems with two significant changes: PROFESS is now parallelized, and the ion–electron and ion–ion terms scale quasilinearly, instead of quadratically as in PROFESS v1 (L. Hung and E.A. Carter, Chem. Phys. Lett. 475 (2009) 163). At the start of a run, PROFESS reads the various input files that describe the geometry of the system (ion positions and cell dimensions), the type of elements (defined by electron–ion pseudopotentials), the actions you want it to perform (minimize with respect to electron density and/or ion positions and/or cell lattice vectors), and the various options for the computation (such as which functionals you want it to use). Based on these inputs, PROFESS sets up a computation and performs the appropriate optimizations. Energies, forces, stresses, material geometries, and electron density configurations are some of the values that can be output throughout the optimization.

New version program summary

Program Title: PROFESS

Catalogue identifier: AEBN_v2_0

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEBN_v2_0.html

Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland

Licensing provisions: Standard CPC licence, <http://cpc.cs.qub.ac.uk/licence/licence.html>

No. of lines in distributed program, including test data, etc.: 68 721

No. of bytes in distributed program, including test data, etc.: 1 708 547

Distribution format: tar.gz

Programming language: Fortran 90

Computer: Intel with ifort; AMD Opteron with pathf90

Operating system: Linux

Has the code been vectorized or parallelized?: Yes. Parallelization is implemented through domain composition using MPI.

RAM: Problem dependent, but 2 GB is sufficient for up to 10,000 ions.

Classification: 7.3

External routines: FFTW 2.1.5 (<http://www.fftw.org>)

Catalogue identifier of previous version: AEBN_v1_0

Journal reference of previous version: Comput. Phys. Comm. 179 (2008) 839

Does the new version supersede the previous version?: Yes

Nature of problem: Given a set of coordinates describing the initial ion positions under periodic boundary conditions, recovers the ground state energy, electron density, ion positions, and cell lattice vectors predicted by orbital-free density functional theory. The computation of all terms is effectively linear

[☆] This paper and its associated computer program are available via the Computer Physics Communications homepage on ScienceDirect (<http://www.sciencedirect.com/science/journal/00104655>).

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scaling. Parallelization is implemented through domain decomposition, and up to $\sim 10,000$ ions may be included in the calculation on just a single processor, limited by RAM. For example, when optimizing the geometry of $\sim 50,000$ aluminum ions (plus vacuum) on 48 cores, a single iteration of conjugate gradient ion geometry optimization takes ~ 40 minutes wall time. However, each CG geometry step requires two or more electron density optimizations, so step times will vary.

Solution method: Computes energies as described in text; minimizes this energy with respect to the electron density, ion positions, and cell lattice vectors.

Reasons for new version: To allow much larger systems to be simulated using PROFESS.

Summary of revisions:

- PROFESS can run in parallel [1]. Parallelization is implemented through domain decomposition using MPI. (However, copies of all ion positions, which take up a relatively small amount of memory, are saved on all processors.) An updated serial version of PROFESS, with some memory-efficient features specific to the use of a single process, can also be compiled from the same code.
- Instead of linking to the FFTW3 library, we use FFTW 2.1.5, which is the most recent version of FFTW that supports MPI parallel transforms.
- Ion–ion and ion–electron calculations can scale as $O(N \ln N)$ through the use of cardinal B-splines [1–3]. (For ion–ion calculations, this is known as particle-mesh Ewald.)
- The line search during electron density optimization (when using the square root of electron density as the variational parameter) automatically conserves the total number of electrons in the system, using a similar line search mixing scheme as in Ref. [4].
- The square root density CG and TN optimizations are generally more stable.
- Conjugate gradient ion optimization is improved and stable.
- Positions of chosen ions can be held fixed during geometry optimization.
- Variable time steps are used during cell lattice optimization instead of fixed steps.
- The CAT kinetic energy density functional [5] is available.
- A cutoff to avoid divergence in vacuum regions is now an option for some kinetic energy and exchange–correlation functionals (keywords WTV, WGV, CAV, PBEC) [6].
- The PBE exchange–correlation subroutine is more stable.
- Calculations of energy and potential for some functionals are more efficient after removing duplicate computations. (Note: CAT, LQ, and HQ functionals have not yet been consolidated.)
- Density and potential output files have a new format that is more convenient for output from multiple processes. A utility to convert between old and new density formats, as well as Tecplot format, is provided in RhoConvert.f90.
- The interpolation scheme used when reading in pseudopotentials is more accurate.
- WGC kernel integration uses the Runge–Kutta method for better accuracy.

Restrictions: PROFESS cannot use nonlocal (such as ultrasoft) pseudopotentials. A variety of local pseudopotential files are available at the Carter group website (<http://www.princeton.edu/mae/people/faculty/carter/homepage/research/localpseudopotentials/>). Also, due to the current state of the kinetic energy functionals, PROFESS is only reliable for main group metals and some properties of semiconductors.

Running time: Problem dependent: the test example provided with the code takes less than a second to run. Timing results for large scale problems are given in the PROFESS paper and Ref. [1].

References:

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