

PROPOSAL FOR AN ESF SCIENTIFIC MEETING

**Efficient density-functional calculations
with atomic orbitals:
a hands-on tutorial on the SIESTA code.**

Organized by

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Abstract.

The SIESTA code has proven to be a very efficient tool for first-principles calculations in materials physics, chemistry, geosciences, and biology. Its efficiency stems, on the one hand, from the use of strictly localized basis sets, and on the other, from the implementation of linear-scaling algorithms which can be applied to suitable systems. A very important feature of the code is that its accuracy and cost can be tuned in a wide range, from quick exploratory calculations to high quality simulations matching the accuracy of plane-wave methods. SIESTA has become very popular and is increasingly being used by people not familiar with *ab-initio* calculations. We propose a five-day hands-on tutorial on the use of the SIESTA code, aimed at researchers from different disciplines who want to use the code and need, apart from basic practice, a grounding on the capabilities of the method and the approximations used. The main goal is that the students can use the code sensibly on their own.

Scientific summary.

Motivation

Electronic structure codes have become mature enough to be used by scientists not trained in the development of the methods themselves. This is a shift away from traditional practice, in which the know-how and the right to use the code was acquired through a long "internship" (a PhD thesis or a postdoc appointment) in one of the groups dedicated to method and code development. Nowadays most codes are distributed with very light licensing restrictions or for affordable fees. While this ease of access is in principle a good thing, it carries the risk of uncritical or poor use of the codes by untrained people. There is thus an increasing demand for training in the sensible use of these methods, with the goal that the prospective user understands the physical and main technical approximations behind a method and can assess its reliability and its usefulness for a particular problem.

In the past few years, the possibility of treating large systems with some first-principles electronic-structure methods has opened up new opportunities in many disciplines, and ever more people not familiar with *ab-initio* calculations are being attracted to these codes. In particular, the SIESTA program (<http://www.uam.es/siesta>) has become quite popular and is increasingly being used by researchers in geosciences, biology, and engineering (apart from the "home base" of materials physics and chemistry). Currently there are more than 800 registered users all over the world (almost 40 are located in Europe, mostly in ESF-member countries), and the paper describing the method [J. Phys.: Condens. Mat. **14** 2745-2779 (2002)] has had more than 500 citations. SIESTA's efficiency stems from the use of strictly localized basis sets and from the implementation of linear-scaling algorithms which can be applied to suitable systems. A very important feature of the code is that its accuracy and cost can be tuned in a wide range, from quick exploratory calculations to highly accurate simulations matching the quality of plane-wave methods.

SIESTA is distributed freely to academics, and a special effort has been made over the years to train people in its use. Previous SIESTA schools [addressing specific communities in Barcelona (1999), Lyon (1999), Rio de Janeiro (2000), Cambridge (2002), Lyon (2003)] were quite popular. The last school, hosted by CECAM, was very successful, with more applicants than could be accommodated, and the demand for a new one is noticeable in the pace of new registrations and the postings to the program's mailing list.

We propose a five-day hands-on tutorial on the use of the SIESTA code, intended for researchers who want to use the code and need, apart from basic practice, a grounding on the capabilities of the method and the approximations used.

Aims

A first aim of the tutorial is to show the students the thread between fundamental laws of physics and the properties of atomic aggregates, and, in so doing, transmit the difficulty of the problem and the essence of the approximations along that thread. Every student should take away: (i) what can be computed, (ii) how to do it, (iii) how good the results can be, and (iv) how bad they can be if things are not done critically and carefully (even if *ab initio*). Apart from the basics of density-functional theory, molecular dynamics simulation and geometry relaxation, which are common to most codes, the specific SIESTA topics to be covered are the generation and use of pseudopotentials, the construction of basis sets of strictly localized numerical atomic orbitals, localization issues for linear scaling both in the computation of the matrix elements and in the resolution of the hamiltonian, as well as more technical ones such as the influence of the real-space grid and parallelization.

Audience

Addressed to young people who plan on using electronic structure methods in their research. Some fundamental knowledge of quantum mechanics will be assumed, as well as basic statistical mechanics for the molecular dynamics part. Some solid state physics background will be helpful but not strictly needed. The basics of these areas will be covered quickly to establish the language. We have decided not to assume any previous *ab-initio* training, as our experience is that many prospective users are interested in self-contained courses. Experts in other electronic structure methods will find most of the lectures of interest, even if the course will feel less intensive for them.

An audience of around 30 would be adequate. For the practical sessions the students will work in pairs on the computer.

Format

Each day there will be morning lectures followed in the afternoon by a practical session. The lectures will be split into: (1) Formal lectures in the early morning, giving the theoretical background and fundamental aspects of the physics and/or methodology of the calculations, and (2) practical lectures in the late morning, with more practicalities related to the implementation and the actual SIESTA usage, preparing for the afternoon session.

Lecturers

The lectures and practical sessions will be conducted by members of the SIESTA development team and very experienced users, and will cover also for the first time post-processing and visualization tools, which are becoming essential.

Most of the members of the SIESTA core team, with the exception of Julian D. Gale and Richard M. Martin, have affiliations within ESF-member countries.

Budget

We would like, at the very least, to cover the room and board expenses of the participants, and the living and travel expenses of the speakers/presenters. We estimate a total budget of 18700 €.

This tutorial is intended to be a Psi-k/CECAM joint activity, and we will submit the corresponding application to CECAM shortly. CECAM's automated budget estimator suggests a sum of 12000 €. We will ask for that amount, but it is likely that we will be granted only around 75% of that sum (around 9000 €), so we will need 10000 € from the ESF.

Funding for participants from the US will be provided by the travel award program of the Materials Computation Center at the University of Illinois Urbana-Champaign. This is already taken into account in the above, as is that two of the presenters might be able to cover their own expenses.

Meeting program.

Day 1:

9:00 Welcome and practical issues.

9:30 Introduction: Computer simulations and their role in research.

10:30 Coffee break —————

11:00 Fundamentals: the quantum-mechanical many-electron problem and the Density Functional Theory approach.

12:00 Brief introduction to SIESTA. What is SIESTA good and efficient for?. Where does it stand in relation to other methods or codes?.

12:30 Introduction to the basic execution of SIESTA (input, output, tools, k-points, SCF...).

13:30 Lunch —————

15:00 Practical session: first runs on simple examples.

16:30 Coffee break —————

17:00 Practical session continued.

Day 2:

9:00 Pseudopotentials.

9:50 Atomic orbitals of finite range as basis sets.

10:40 Coffee break —————

11:10 How to generate and test pseudopotentials (including dealing with partial core corrections and semicore states).

12:00 How to generate and test basis sets.

13:00 Lunch —————

15:00 Practical session: preparing and testing pseudopotentials and basis sets. Transferability and hardness of the pseudopotential. Quality and transferability of the basis set.

16:30 Coffee break ———

17:00 Practical session continued.

Day 3:

9:00 Code structure: calculation of matrix elements of H and S. Direct diagonalization.

9:40 Linear scaling fundamentals and algorithms.

10:40 Coffee break ———

11:10 How to run with linear-scaling solvers.

12:00 Systematic convergence for realistic projects: from Quick & Dirty to converged calculations. Converging the calculation with mesh-cutoff, k-point sampling, and size and range of the basis set.

13:00 Lunch —————

15:00 Practical session: a realistic problem. Linear scaling.

16:30 Coffee break ———

17:00 Practical session continued.

Day 4:

9:00 Molecular Dynamics (MD) in different ensembles. Geometry relaxations and calculation of vibrational spectrum.

9:45 The parallelization of SIESTA.

10:30 Coffee break ———

11:00 Practicalities about using Molecular Dynamics.

12:00 Compiling and running in parallel.

13:00 Lunch —————

15:00 Practical session: a realistic problem. MD / use of the Vibra suite.

16:30 Coffee break ———

17:00 Practical session continued.

Day 5:

9:00 Calculation of optical properties. Calculation of polarization properties of insulators.

10:00 Introduction to TRANSIESTA (calculation of transport properties).

11:00 Coffee break ———

11:30 Visualization and post-processing tools. Plotting the charge density, wave functions, Fermi surface, etc. Analyzing MD runs.

13:00 And now that you are back at home... what?. Licenses and how to get the SIESTA code. Compilation issues.

13:30 Lunch —————

15:00 Practical session: a realistic problem. Computation of optical and polarization properties. Examples on visualization tools. Free projects.

16:30 Coffee break ———

17:00 Practical session continued.

Curricula of scientific organizers.

Javier Junquera

Born in Córdoba (Córdoba, Spain) on 31 May 1974

Current appointment

Ramón y Cajal fellow,
Departamento de Ciencias de la Tierra y Física de la Materia Condensada
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Research lines

First-principles calculations in Condensed-Matter Physics. Size effects on ferroelectric materials. Surface and interfaces phenomena. High- κ materials. Development of scientific computing codes.

Education

- Licenciado en Ciencias Físicas, Universidad de Oviedo, Spain (September 1996)
- Doctor en Ciencias Físicas, Universidad Autónoma de Madrid (advisors: P. Ordejón and E. Artacho) (September 2001)

Former appointments

- Sep 96-Mar 99
PhD student, Departamento de Física,
Universidad de Oviedo, Spain.

- Mar 99-Sep 99
Profesor Asociado (Teaching Assistant), Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain.
- Sep 99-Sep 01
Ayudante (Assistant Professor), Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain.
- Sep 01-Aug 03
Assistant, Département de Physique, Université de Liège, Belgium.
- Aug 03-Sep 04
Postdoctoral Associate, Department of Physics and Astronomy, Rutgers University, New Jersey, USA.

Most relevant publications in the past five years

- J. Junquera, Ó. Paz, D. Sánchez-Portal, and E. Artacho, “Numerical atomic orbitals for linear-scaling calculations”, *Phys. Rev. B* **64** 235111 (2001). Times Cited: 79
- J. M. Soler, E. Artacho, J. D. Gale, A. Garcia, J. Junquera, P. Ordejón, D. Sánchez-Portal, “The SIESTA method for ab initio order- N materials simulation”, *J. Phys.: Condens. Matter* **14**, 2745-2779 (2002). Times cited: 548
- J. Junquera and Ph. Ghosez, “Critical thickness for ferroelectricity in perovskite ultrathin films” *Nature* **422**, 506-509 (2003). Times cited: 125
- J. Junquera, M. Zimmer, P. Ordejón, and Ph. Ghosez, “First-principles calculation of the band offset at BaO/BaTiO₃ and SrO/SrTiO₃ interfaces” *Phys. Rev. B* **67**, 155327 (2003). Times Cited: 12
- C. Lichtensteiger, J.-M. Triscone, J. Junquera, and Ph. Ghosez, “Ferroelectricity and tetragonality in ultrathin PbTiO₃ films”, *Phys. Rev. Lett.* **94** 047603 (2005). Times Cited: 18
- “First-Principles Modeling of Ferroelectric Oxides Nanostructures”, Ph. Ghosez and J. Junquera, in “Handbook of Theoretical and computational nanotechnology”, Ed. by M. Rieth and W. Schoomers, (American Scientific Publisher, Stephenson Ranch, CA, USA, 2006). Review containing more than 100 pages, 61 figures, and 384 references.

Recent Invited Talks

1. “Ferroelectric properties of Ultrathin Perovskite Heterostructures” March Meeting of the APS, Montreal (Canada), March 2004.
2. “A new proposal for a XML-based unified pseudopotential format”, Twelfth International Workshop on Computational Physics and Material Science: Total Energy and Force Methods, Trieste (Italy), January 2005.
3. “First-principles computations on size-effects in epitaxial ferroelectric heterostructures”, 230th American Chemical Society (ACS) National Meeting, Washington DC (USA), August 2005.
4. “Interface effects in ferroelectric thin-film devices”, Psi-k 2005 Conference, Swäbisch-Gmünd (Germany), September 2005.

5. “First-principles computations on size-effects in epitaxial ferroelectric heterostructures”, Fall Meeting of the Material Research Society (MRS), Boston (USA), December 2005.
6. “A proposal for a unified norm-conserving pseudopotential format”, Data representation and code interoperability for computational material physics and chemistry, Lyon (France), April 2006.

Organization of research activities

- Co-organizer of the SIESTA School (Linear-Scaling LCAO Program) July 2002 (Cambridge, UK).
- Lecturer in the “International Workshop in Computational Materials Science”, May 2005 (Lanzhou, China).
- Organizer of the SIESTA Meeting, April 2006 (Santander, Spain).

Other

- According to the ISI Web of Knowledge (September 22, 2006):
Total number of citations: 1088
Average number of citations per article: 52
Most cited paper (not first author): 548
Most cited paper (first author): 125
- Active referee in Nature, Physical Review Letters, Physical Review B, Europhysics Letters, Journal of Physics D: Applied Physics, Applied Surface Science, Material Research Society Symposium Proceedings.
- The paper published in Nature was chosen as highlight of the week.
- Some of my first works, done under the auspices of Motorola INC, were used to patent the manufacturing process of the (by that time) smallest transistor in the world.

Alberto García

Born in Baracaldo (Vizcaya, Spain) on 23 August 1963

Current appointment

Staff Scientist,
Instituto de Ciencia de Materiales de Barcelona - CSIC
Campus de la UAB – Bellaterra 08193 (Barcelona)
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FAX: (+34) 935.805.729,
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Research lines

First-principles calculations in Condensed-Matter Physics. Simulations with effective Hamiltonians. Phase transitions. Ferroelectricity. Development of scientific computing codes.

Education

- Licenciado C. Físicas, Universidad del País Vasco, Spain (June 1986)
(First National Prize)
- Ph.D. Physics, U.C. Berkeley (advisor: Marvin L. Cohen) (September 1992)

Former appointments

- Sep 86-Jul 87
PhD student, Departamento de Física
Universidad del País Vasco
- Aug 87-Sep 92
PhD student, Department of Physics
University of California, Berkeley, USA
- Oct 92-Sep 94
Postdoctoral researcher, Eletronic Materials Laboratory
Xerox Palo Alto Research Center
Palo Alto, California, USA
- Oct 94-Feb 95
Postdoctoral researcher, Department of Physics and Astronomy
Rutgers University
Piscataway, New Jersey, USA
- Feb 1995-Jun 2006
Professor (tenured since 1998) Facultad de Ciencias, Universidad del Pas Vasco

Summary of research accomplishments

- Over 50 publications in peer-reviewed journals, with over 1600 citations.
- Supervision of two doctoral dissertations, with another in progress.

Most relevant publications in the past five years

- J. Íñiguez, S. Ivantchev, A. García, J. M. Pérez-Mato, “Devonshire-Landau free-energy of BaTiO₃ from First Principles”, *Phys. Rev. B* **63**, 144103 (2001).
- L. Bellaiche, Alberto García, and David Vanderbilt, “Electric-field induced polarization paths in Pb(Zr_{1-x}Ti_x)O₃ alloys,” *Phys. Rev. B* **64**, 060103 (2001).
- D. Sánchez-Portal, J. D. Gale, A. García, and R. M. Martin, “Si(557)-Au surface: monatomic Au wires displaying two metallic bands”, *Phys. Rev. B* **65**, 081401 (2002).
- J. M. Soler, E. Artacho, J. D. Gale, A. García, J. Junquera, P. Ordejón, D. Sánchez-Portal, “The SIESTA method for ab initio order-*N* materials simulation”, *J. Phys.: Condens. Matter*, **14**, 2745-2779 (2002). (548 citations)
- J. M. Pérez-Mato, M. I. Aroyo, A. García, P. Blaha, K. Schwarz, J. Schweifer and K. Parlinski, “Competing structural instabilities in the ferroelectric Aurivillius compound Bi₂SrTa₂O₉”, *Phys. Rev. B* **70**, 214111, (2004)
- I. Etxebarria, J. M. Pérez-Mato, A. García, P. Blaha, K. Schwarz, and J. Rodriguez-Carvajal, “A comparison of empirical bond-valence and first-principles energy calculations for a complex structural instability” *Phys. Rev. B* **72**, 174108 (2005).

Recent Invited Talks

1. “Recent developments in ab-initio calculations in ferroelectrics with effective hamiltonians”, 10th International Meeting of Ferroelectricity, Madrid (September 2001).
2. “Simulation of effective Hamiltonians: new views of ferroelectric behavior”, Symposium on Nano-sized Materials, University of Liege (Belgium) (December 2002).
3. “An XML parser in Fortran”, CECAM workshop on “Software solutions for data exchange and code gluing”, Lyon, France (October 2003).
4. “A native Fortran XML parser: Design and applications in scientific computing”, NeSC workshop “Toward a common data and command representation for quantum chemistry”, National e-Science Institute, Edinburgh, UK (April 2004).
5. “Software tools for data interchange”, Twelfth International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, Trieste, Italy (January 2005).

Organization of research activities

- Co-organizer of the ‘Workshop on Advances in First-Principles Computational Condensed Matter Physics’, (Miraflores de la Sierra (Madrid)), 2000
- Co-organizer of the series of SIESTA Schools (Linear-Scaling LCAO Program) July 2002 (Cambridge, UK) , December 2003 (Lyon, France)

- Co-organizer of the CECAM-Psi-k workshop “Data representation and code interoperability for computational materials physics and chemistry” (April 2006)

Other

- Extensive experience in scientific computing, including programming languages, mathematical libraries, data storage and visualization, parallel-computing techniques, and operating-system administration.
- At one point or another, maintainer of several major scientific computing codes: ATOM, PW, CUSP, SIESTA, MC. Very good command of source control techniques and other software engineering concepts.
- Design and development of a flexible interface for data input in Fortran programs (FDF (Flexible Data Format), with José Soler).
- Design and development of a Fortran XML parser (XMLF90)
<http://fisica.ehu.es/ag/xml/>
- Member of the steering committee of the FSAtom project on open-source software for atomic-level simulations.
- Member of the steering committee of the University’s Scientific Computing Services.

Provisional list of proposed speakers and participants.

Provisional list of proposed lecturers.

- Javier Junquera (Universidad de Cantabria, Spain).
- Alberto García (ICMAB, Barcelona, Spain).
- Pablo Ordejón (ICMAB, Barcelona, Spain).
- Daniel Sánchez-Portal (DIPC, San Sebastian, Spain).
- Emilio Artacho (Cambridge University, UK).
- Andrei Postnikov (Paul Verlaine University, Metz, France).
- Richard M. Martin (University of Illinois, Urbana-Champaign, USA).
- Julian D. Gale (Curtin University of Technology, Perth, Australia).

Proposed participants

As this proposal refers to a tutorial, we do not have advance information about the participants.