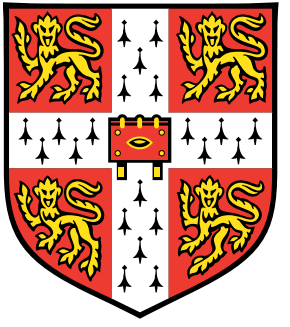
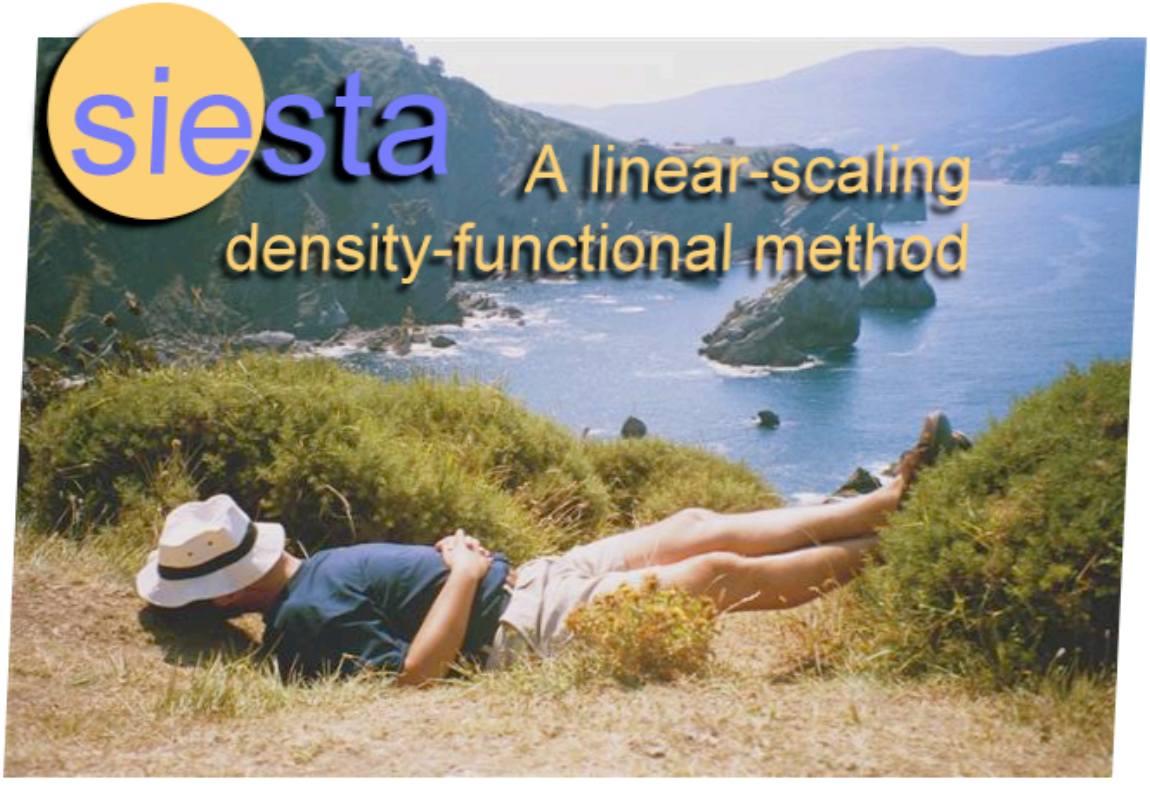
What next?

Toby White
Dept. Earth Sciences, University of Cambridge





http://www.uam.es/siesta/

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- 1. *Self-consistent order-N density-functional calculations for very large systems*, P. Ordejón, E. Artacho and J. M. Soler, Phys. Rev. B (Rapid Comm.) **53**, R10441 (1996).
  2. *The Siesta method for ab initio order-N materials simulation*, José M. Soler, Emilio Artacho, Julian D. Gale, Alberto García, Javier Junquera, Pablo Ordejón and Daniel Sánchez-Portal, J. Phys.: Condens. Matter **14**, 2745 (2002).

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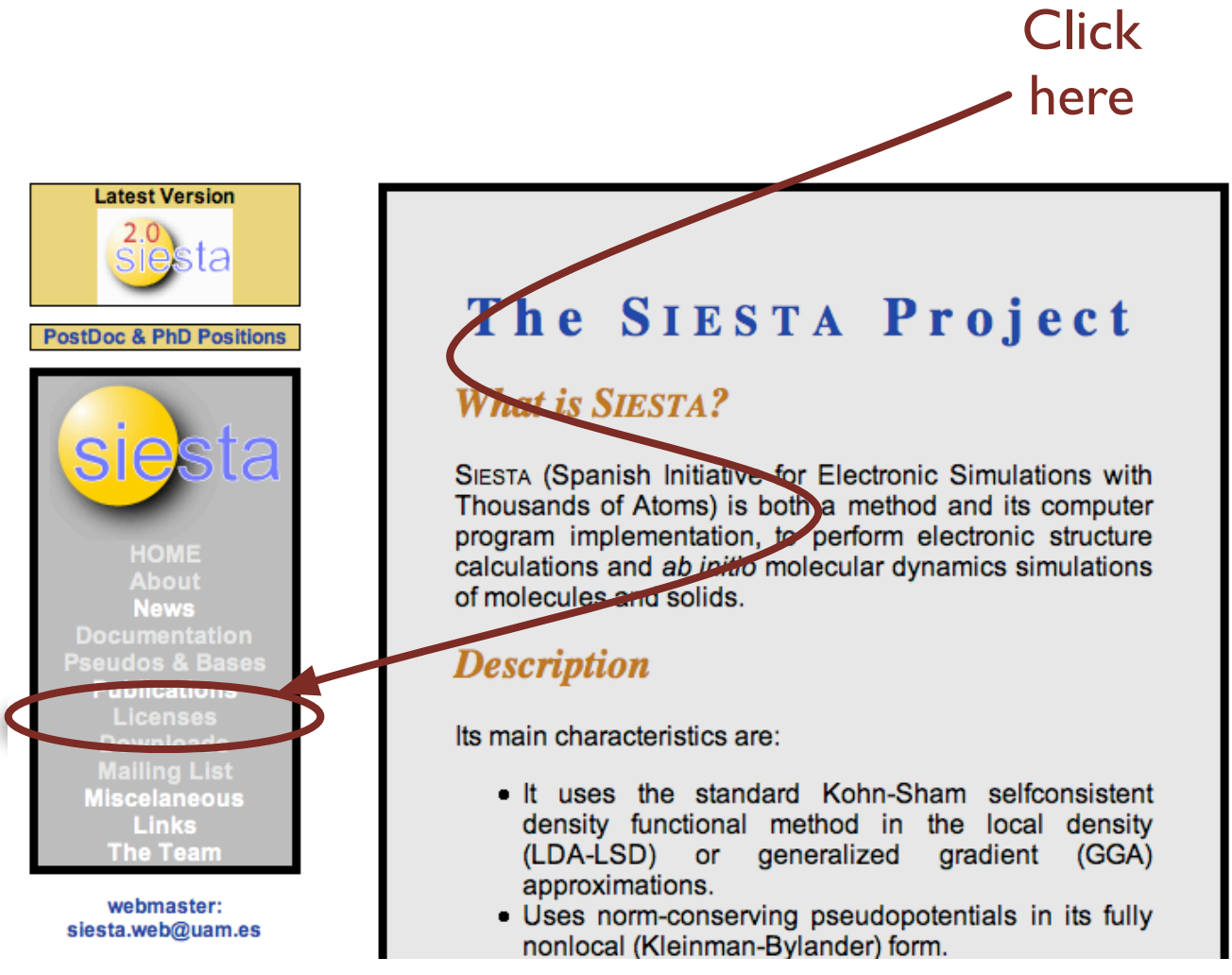
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The SIESTA Project
What is SIESTA?
SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) is both a method and its computer program implementation, to perform electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids.
Description
Its main characteristics are:
It uses the standard Kohn-Sham selfconsistent density functional method in the local density (LDA-LSD) or generalized gradient (GGA) approximations.
Uses norm-conserving pseudopotentials in its fully nonlocal (Kleinman-Bylander) form.


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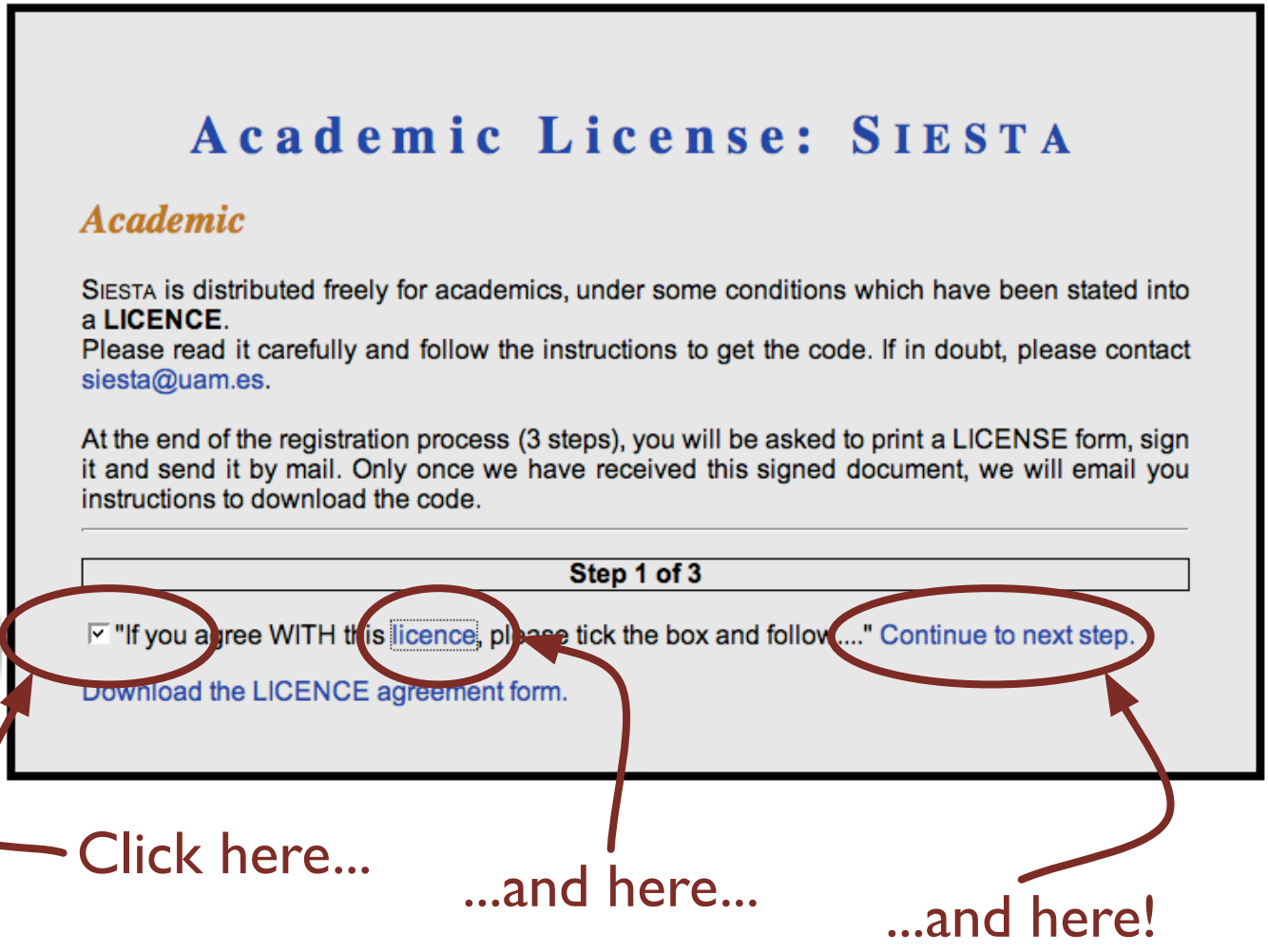
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SIESTA ACADEMIC LICENCE for INDIVIDUALS

Motivation and Preamble

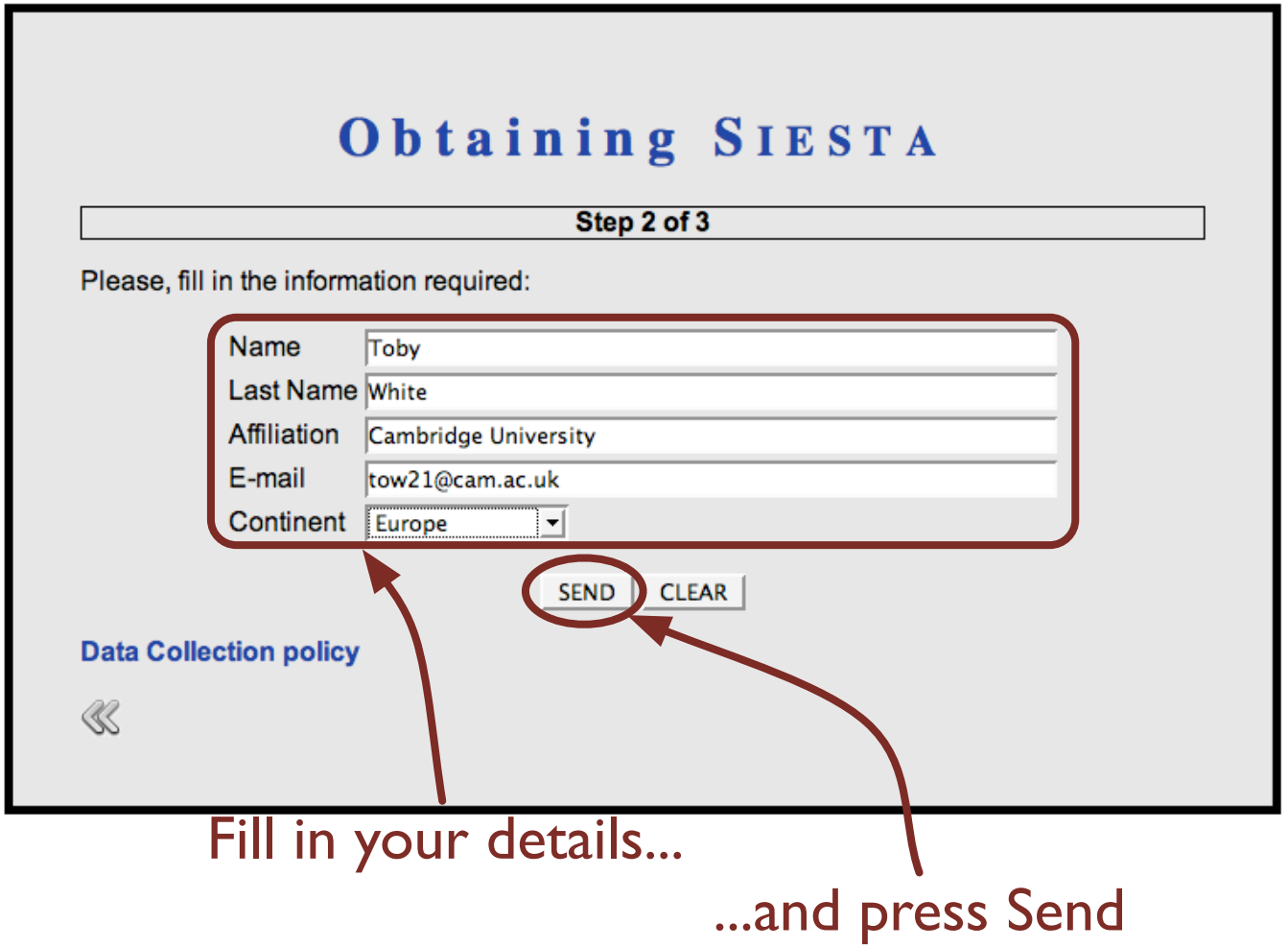
The SIESTA program has been devised for its general use in research within the academic community. Some conditions have been defined for the use, distribution, and modification of SIESTA, which the authors consider fair and within the common fair practices in the academic community.

1. Definitions

"The Authors" are:

- Emilio Artacho, University of Cambridge
- Julian Gale, Curtin University of Technology, Perth
- Alberto García, Universidad del País Vasco, Bilbao
- Javier Junquera, Rutgers University
- Pablo Ordejón, ICMAB-CSIC, Barcelona
- Daniel Sánchez-Portal, Universidad del País Vasco, San Sebastián
- José M. Soler, Universidad Autónoma de Madrid

Although we, the Authors, acknowledge that a limited number of auxiliary subroutines were written by (or are based on previous subroutines written by) other authors consider that the implementation of all the basic algorithms of the SIESTA program is ours.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Step 2 of 3
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Last Name
White
Affiliation
Cambridge University
E-mail
tow21@cam.ac.uk
Continent
Europe
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CLEAR
Data Collection policy
Fill in your details...
...and press Send

Obtaining SIESTA

Step 3 of 3

Download the SIESTA LICENCE (PDF file) and send **one signed** hard copy to:

Patricia Álvarez c/o Pablo Ordejón
Instituto de Ciencia de Materiales de Barcelona, CSIC
Campus de la UAB
08193 Bellaterra
Barcelona
Spain

Download the LICENCE

Once we receive your signed LICENSE, we will send you an email with instructions to download the package.

Thank you, Toby White

Sign the license and
PUT IT IN THE POST!

❖ *Sign up to mailing list*

Email to: LISTSERV@LISTSERV.UAM.ES

no subject, contents:

```
SUBSCRIBE SIESTA-L your_name
```

Receive confirmation ...
Email again:
no subject, contents:

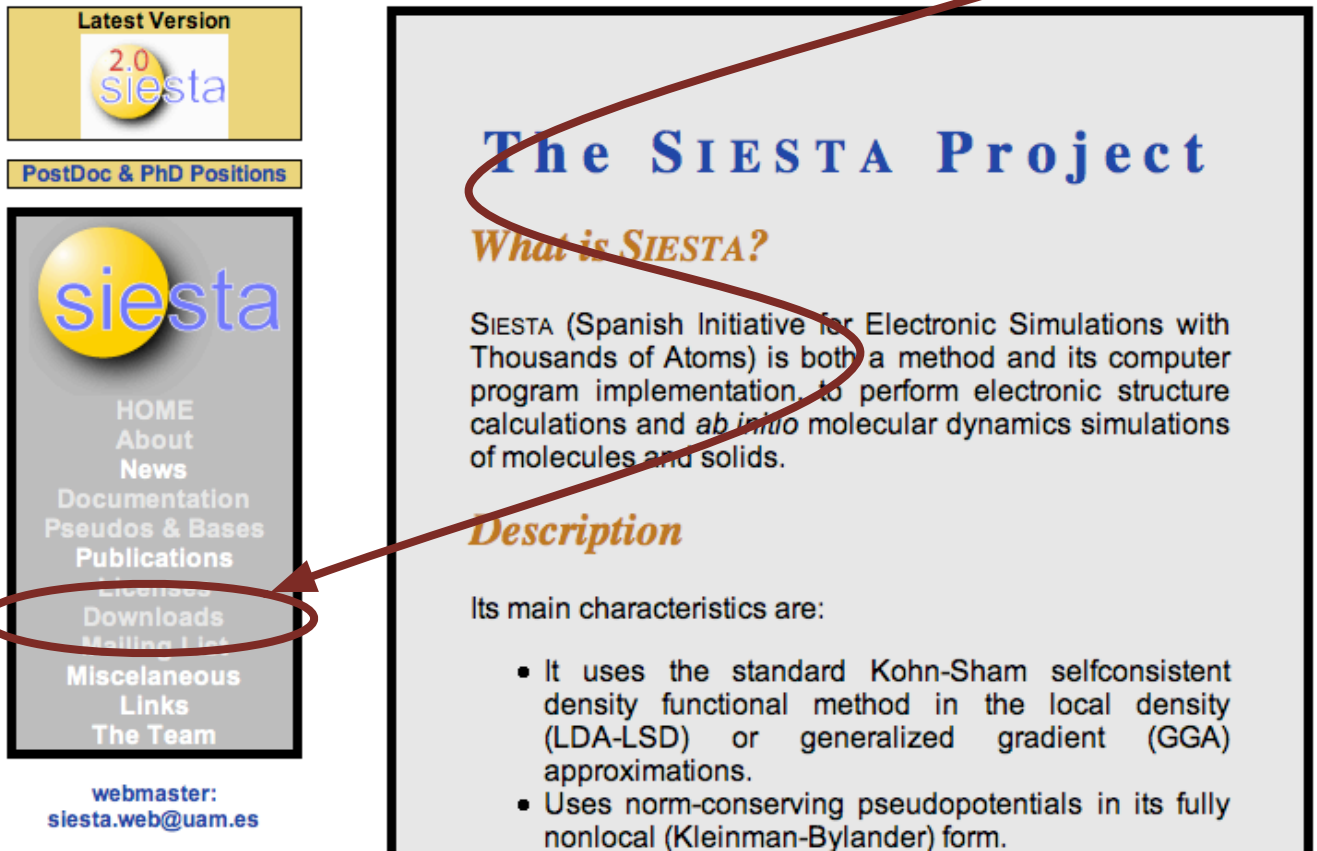
```
PW ADD your_password
```

Read archives at:

http://listas.uam.es/archives/siesta-l.html

❖ Get source code

Click here



❖ Compile Siesta

Parallel compilation hard - use mailing list (and notes from lecture)

Serial compilation much easier!

```
./configure && make
```

```
mkdir iFort_test_1;
cd iFort_test_1;
export srcdir=../Src
$srcdir/configure
```

```
$srcdir/configure --enable-fast
```

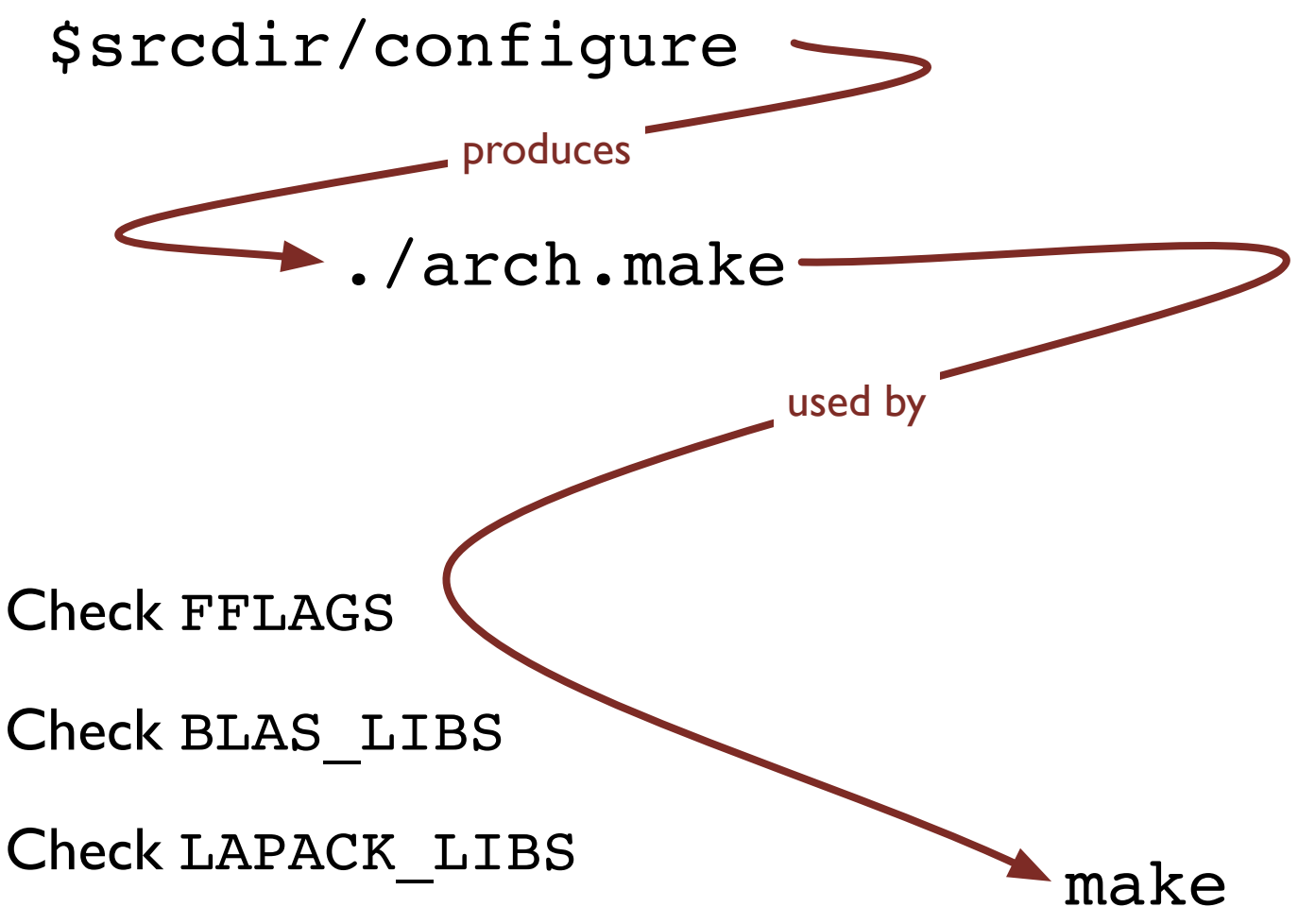
Rough guesses at optimizing flags - always experiment further

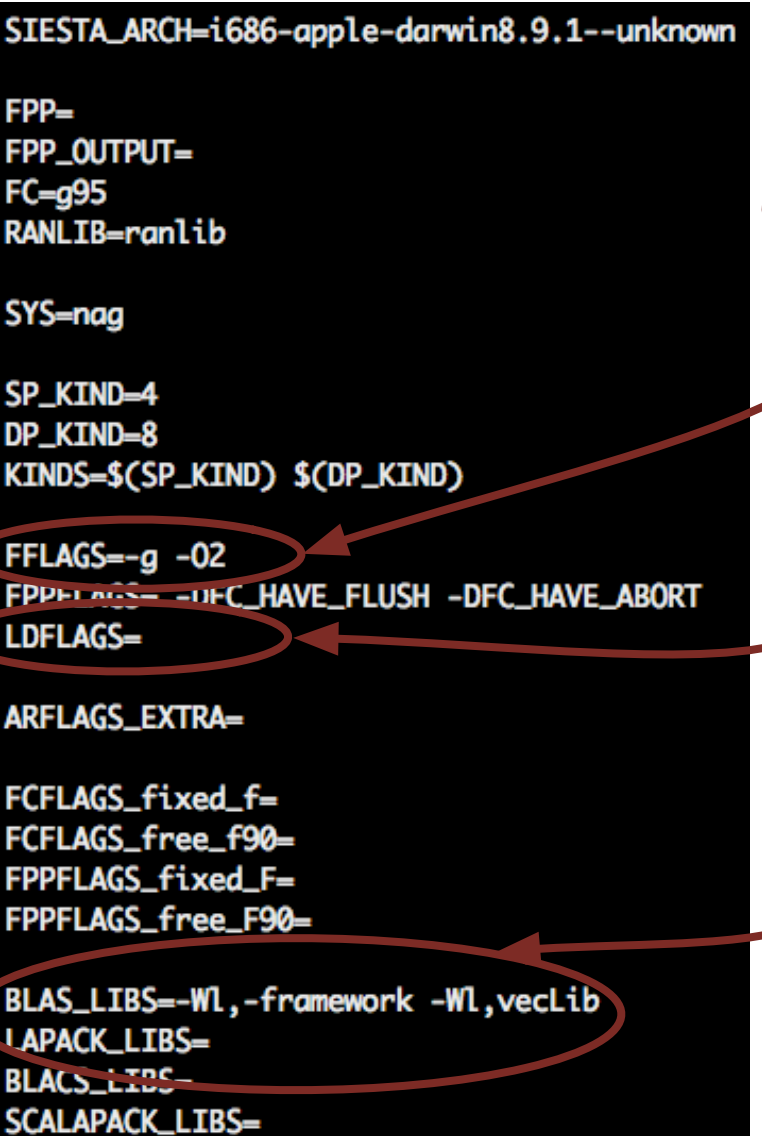
```
$srcdir/configure --enable-debug
```

Very useful if developing - do not use for real runs

```
$srcdir/configure FC=/path/to/f95
```

If more than one compiler is installed, or `configure` can't find the one you want.

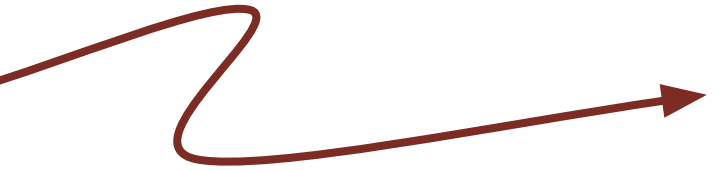

$srcdir/configure
produces
./arch.make
used by
Check FFLAGS
Check BLAS_LIBS
Check LAPACK_LIBS
make



Compiler flags for optimization

Linking flags; `-static` ?

vendor-optimized BLAS/LAPACK



Test the executable.

- `Tests` directory:
  includes test jobs & correct output.

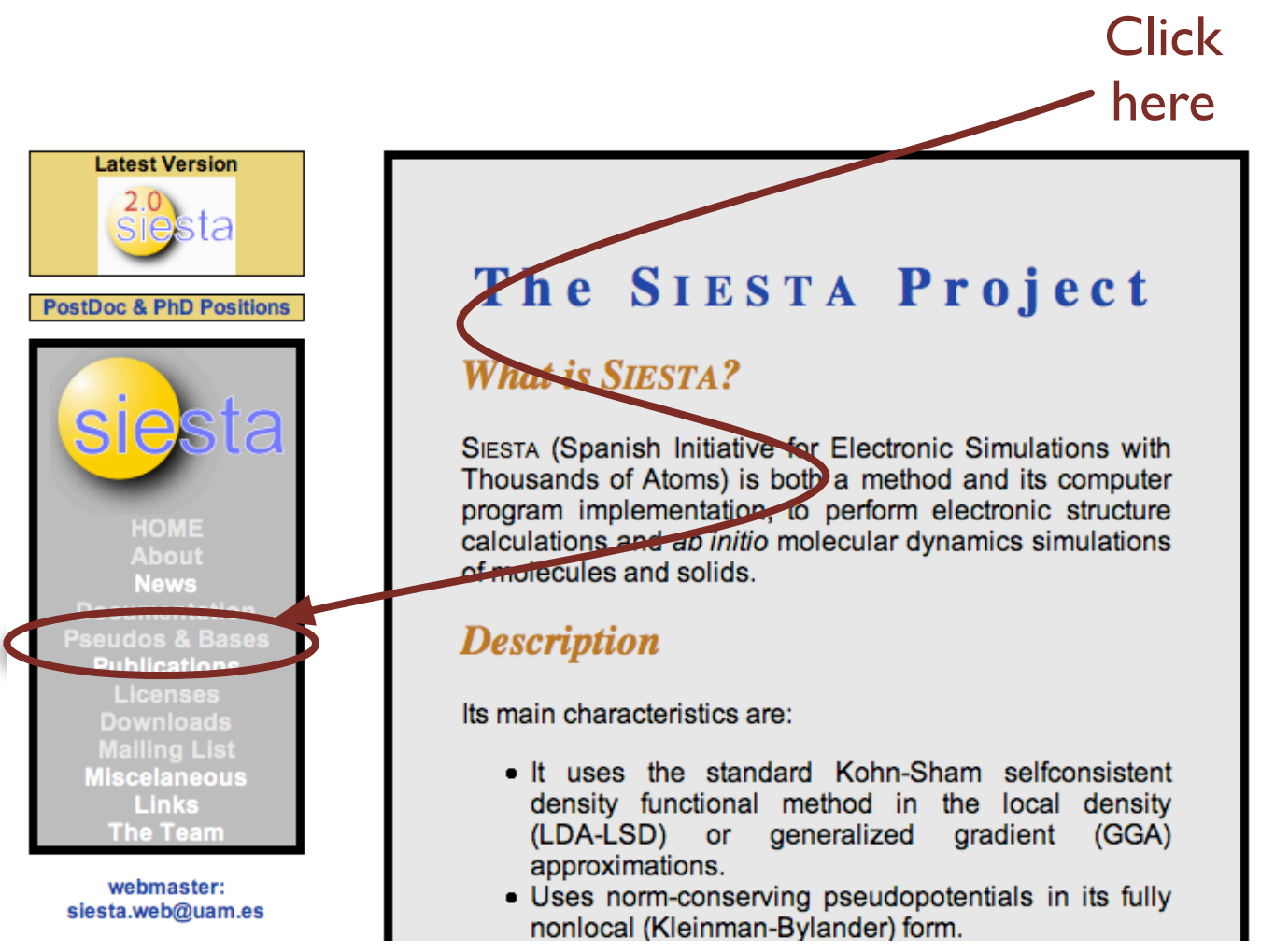
May not work on another computer.
You might need a *static* executable.

❖ *Getting pseudos and basis sets*

Generate them (see lecture and practical session)

Ask on mailing list

Check the database!!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• Uses norm-conserving pseudopotentials in its fully nonlocal (Kleinman-Bylander) form.

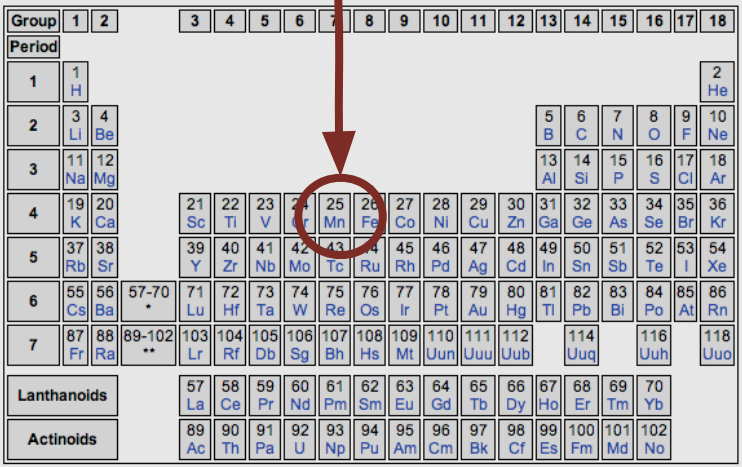
Pick your element

Pseudopotential and Basis Database

Tool devised for the sharing of pseudopotentials and basis sets within the SIESTA community

Use at own risk. Neither the SIESTA team nor the person uploading are responsible for the suitability of uploaded material for your particular problem. The SIESTA team does not test pseudos or bases that are uploaded. Pseudopotentials and basis sets should always be tested in well-known situations, before using them for predictions.

(The pseudo and basis for Ti uploaded by J. Junquera or the ones for Mn by Miguel Pruneda and Valeria Ferrari can be used as example uploads).



Available pseudopotentials:

Mn.3s3p.PCC (Author: Miguel & Valeria; created on 13/10/2005)

Manganese (Mn+2) with 3s and 3p orbitals as semicore, and partial core corrections (PCC). Notice that this is the ionic configuration, without 4s electrons!!

Mn.3s3p (Author: Mn 3s3p ; created on 13/10/2005)

Manganese (Mn+2) with 3s and 3p as semicore, and PCC

Available basis sets:

Mn.3s3pPCC (Author: Valeria & Miguel; created on 13/10/2005)

Basis set (with the new scheme for confinement) used for LaMnO3. Single Zeta (SZ)description is used for semicore orbitals (3s & 3p), and Double Zeta for 4s and 3d. An additional 4p orbital (SZ) is used as polarization for the 4s.

Mn: pseudopotentials

Mn.3s3p.PCC (created 13/10/2005)

Author: Miguel & Valeria (email author)

(Input file)

Manganese (Mn+2) with 3s and 3p orbitals as semicore, and partial core corrections (PCC). Notice that this is the ionic configuration, without 4s electrons!!

Tests:

```
The tests of transferability (as in atom's manual) are better for electronic exci
Electronic excitation's energies (non-spin polarized):
All-electron:
 &d total energy differences in series
 &d          1         2         3         4
 &d  1    0.0000
 &d  2    2.4126    0.0000
 &d  3   -1.2873   -3.6999    0.0000
 &d  4   -1.7230   -4.1356   -0.4357    0.0000
PSEUDOPOTENTIAL:
 &d          1         2         3         4
 &d  1    0.0000
 &d  2    2.4136    0.0000
 &d  3   -1.2862   -3.6998    0.0000
 &d  4   -1.7198   -4.1334   -0.4336    0.0000
Reference Systems:
 ATM3      1         Mn+2 -- Ground State                              &v&d
```

Mn: basis set

Basis: Mn.3s3pPCC (created 13/10/2005)

Author: Anonymous (email author)

(Basis file)

Description:

```
Basis set (with the new scheme for confinement) used for LaMnO3.  Single Zeta (SZ d
```

Tests:

```
Tests done for the cubic-phase of LaMnO3 (using the pseudo & basis for La.+3 in the

Lattice constant (Ang)      Magnetic Moment
    3.847                       3.625
    3.934 (exp)                 3.996

The experimental value for the lattice constant is obtained from the experimental v
```

References:

Associated pseudopotential:

Mn3s3pPCC

❖ Other resources

Andrei Postnikov's utilities (and see his talk and exercises)
http://www.home.uni-osnabrueck.de/apostnik/download.html

Lev Kantorovich
http://www.cmmp.ucl.ac.uk/~lev/codes/lev00/index.html

CMLComp (and see talk and exercises on SIESTA XML)
http://cmlcomp.org

GDIS
http://gdis.sf.net

Scispace.net

http://scispace.net/