



User support in the SIESTA ecosystem

Mónica García Mota (Simune Atomistics SL)



USER SUPPORT IN THE SIESTA ECOSYSTEM



USER SUPPORT

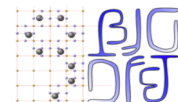


MaX USERS' SUPPORT SERVICES



- ❖ Support for MaX codes and beyond (supporting also some other codes in material science area)
- ❖ **High level consultancy:** support end-users and communities by direct consulting and ad-hoc solutions, possibly comprising codes development and refactoring

<http://www.max-centre.eu/services>



Examples of MaX support actions

- Investigation of **the possible causes of a job failure and solution** of the related problems
- Evaluation of the **MaX codes performance on different architectures**
- Analysis of MaX codes anomalies wrt documentation (e.g. non-converging algorithms)
- **Debugging of problems due to a specific code implementation** (e.g. GPU, MPI, OpenMP versions)
- Selection of the best code parameters that minimize the time to achieve a converged solution
- Optimization of the computational setup to **maximize the performance of a certain simulation on a given architecture** (e.g. find the best combination of number of nodes, number of cores, number of mpi processes/threads, etc...)
- Support in the usage of different **releases of MaX codes** (user guidance about new vs deprecated features)

MaX USERS' SUPPORT SERVICES



Support offered in **two different ways**:

- **by each code community via forum/ mailing lists**, where the responsible is always a specialist acting on behalf of MaX;



https://departments.icmab.es/leem/SIESTA_MATERIAL/Docs/list.html

- **via the MaX Help-desk operated by Cineca**
for each request a ticket is opened in a queue dedicated to MaX.



HELP DESK

support@max-centre.eu

SIMUNE & SIESTA-PRO PROJECT

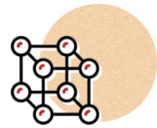


SIMUNE was launched in 2014 as a joint venture of developers of SIESTA* and ANT** codes, and Nanoscience Cooperative Research Center CIC nanoGUNE.

* Pablo Ordejon, Emilio Artacho and Jose Soler

**Juan José Palacios

SERVICES:



Material Design



Code Support
Program



SIESTA Support

PRODUCT:



ATOMISTIC SIMULATION ADVANCED PLATFORM

SIMUNE & SIESTA-PRO PROJECT



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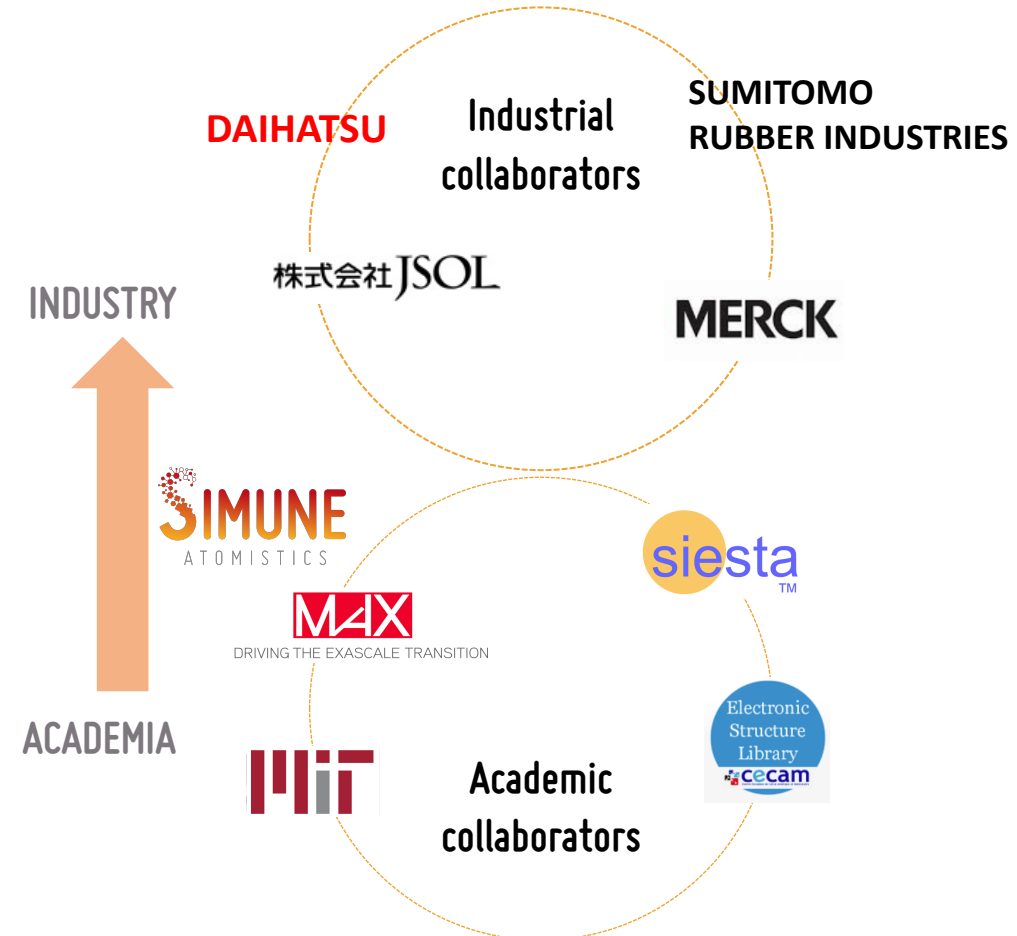
* Pablo Ordejon, Emilio Artacho and Jose Soler

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SERVICES:



PRODUCT:



SIMUNE & SIESTA-PRO PROJECT



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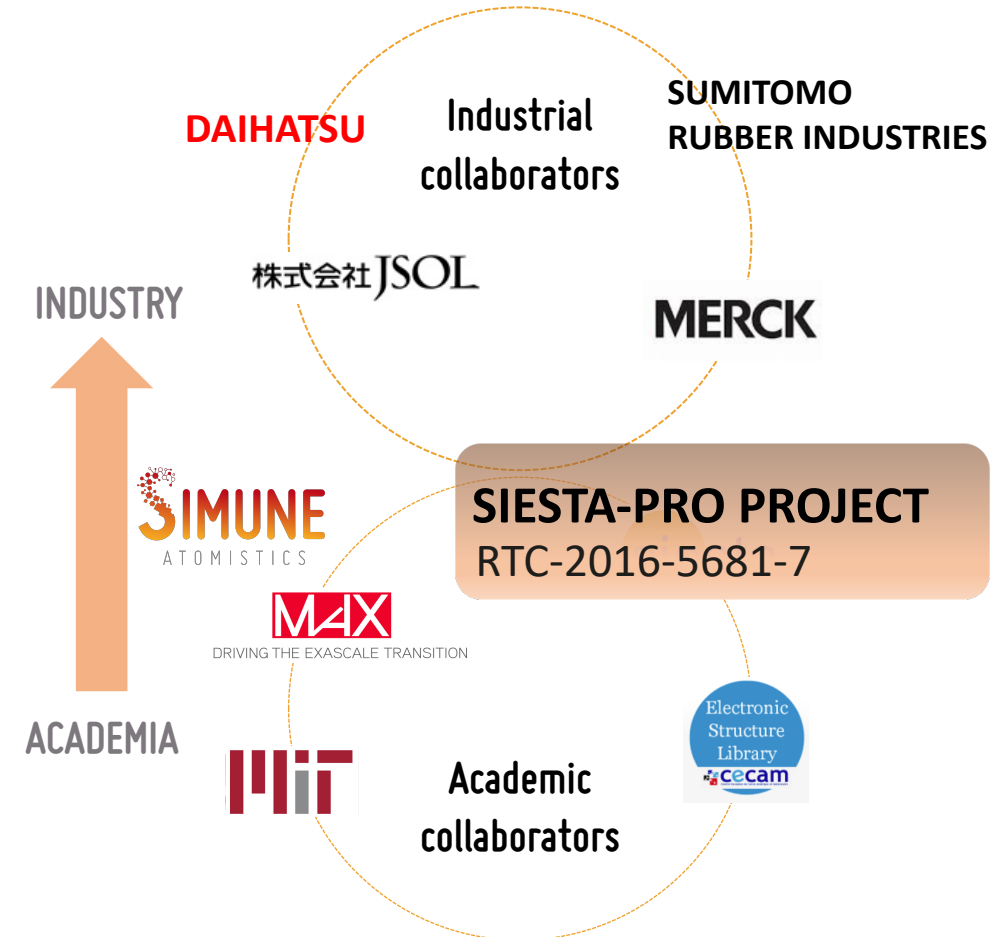
* Pablo Ordejon, Emilio Artacho and Jose Soler

**Juan José Palacios

SERVICES:



PRODUCT:



SIESTA-PRO PROJECT

SIESTA-PRO – Spanish Initiative for Electronic Simulations with Thousands of Atoms: Open Source code with professional support and warranty (2016-2020)

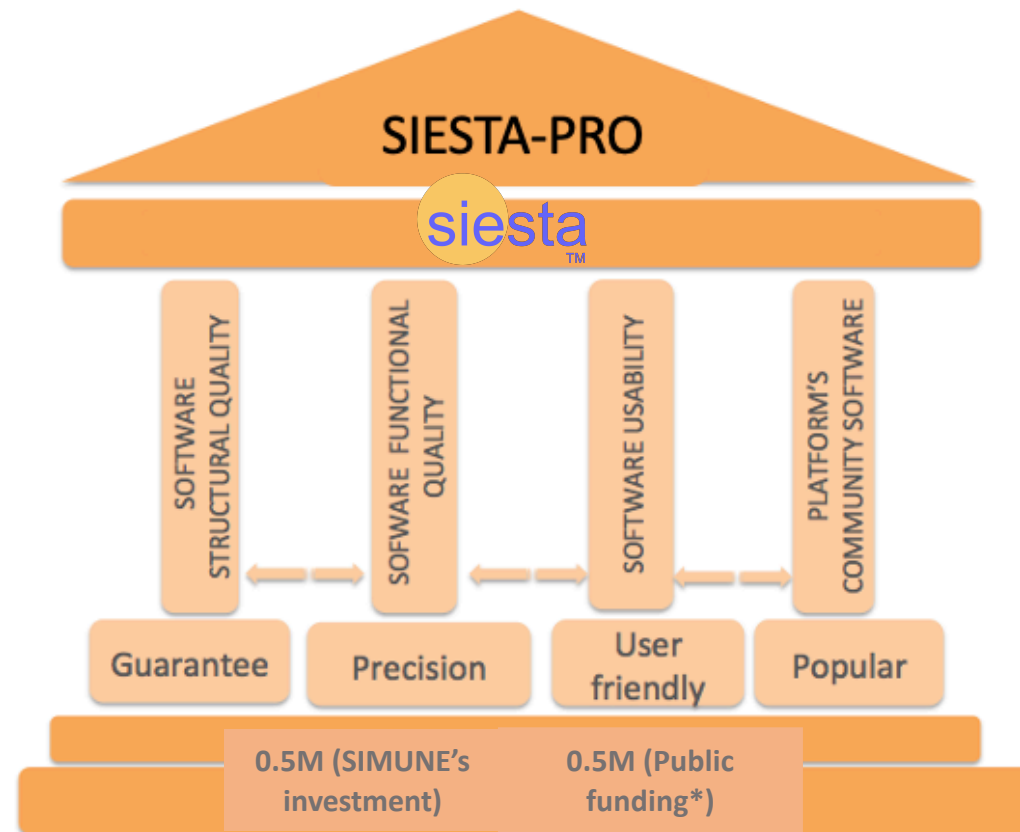
Project partners:

SIMUNE (project coordinator)

UC: Y. Pouillon & J. Junquera

CSIC-CFM: P. Tarifa & D. Sanchez-Portal

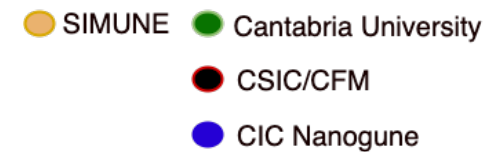
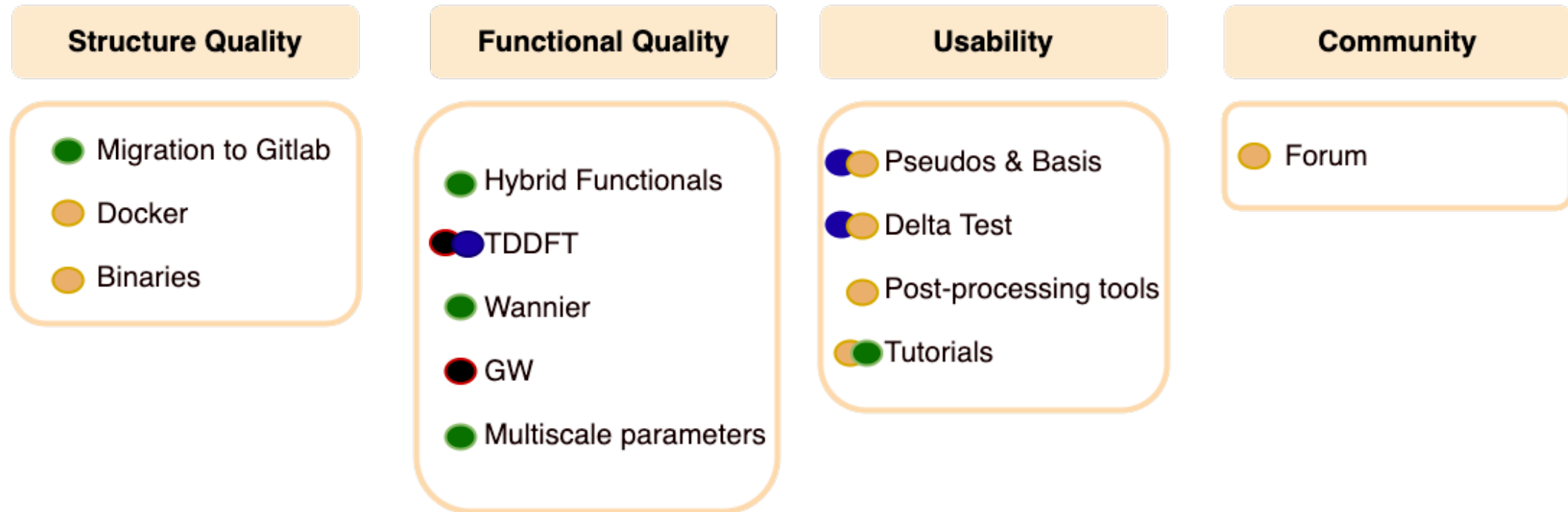
CIC NanoGune: D. Lopez & E. Artacho



*The project (RTC-2016-5681-7) has been funded by the Spanish Ministry of Economy, Industry and Competitiveness and has been co-financed by the European Structural and Investment Funds with the objective to promote technological development, innovation and quality research.

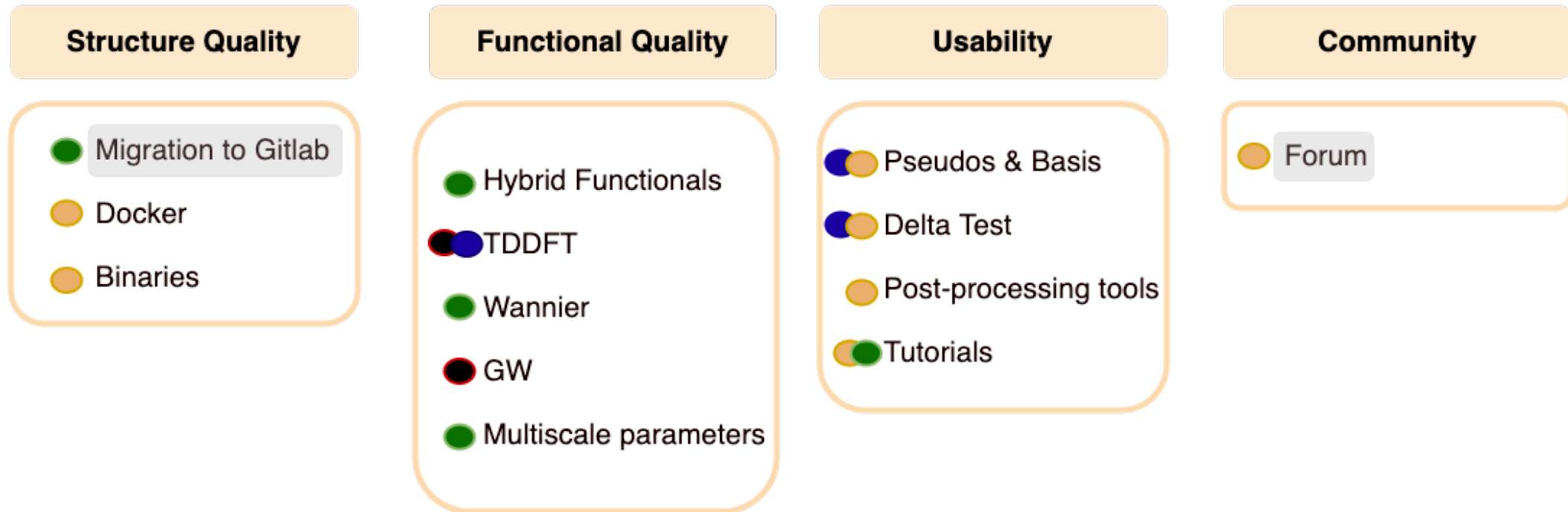
SIESTA-PRO PROJECT

Deliverables:



SIESTA-PRO PROJECT

Deliverables:



- SIMUNE
- Cantabria University
- CSIC/CFM
- CIC Nanogune

SIESTA COMMUNITY

Migration to Gitlab:

The screenshot shows the GitLab interface for the 'siesta' project. The top navigation bar includes 'GitLab', 'Projects', 'Groups', 'Snippets', and 'Help', along with a search bar and 'Sign in / Register' link. The left sidebar contains navigation options: Project overview, Details (selected), Activity, Releases, Repository, Issues (24), Merge Requests (11), Requirements, CI / CD, Security & Compliance, Operations, Packages & Registries, Analytics, Wiki, Snippets, and Members.

The main content area displays the project details for 'siesta' (Project ID: 10326616). It shows 4,455 Commits, 5 Branches, 48 Tags, 10.8 MB Files, 12.6 MB Storage, and 4 Releases. A recent commit is highlighted: 'maint: upgraded lapack for missing routines' by Nick R. Papior, authored 4 days ago, with commit ID b4400266. Below this, there are links for 'README' and 'GNU GPLv3' license.

Name	Last commit	Last update
.gitlab	[admin]: Add BugReport and Suggestion is...	2 months ago
Docs	Merge branch 'rel-4.1'	4 days ago
Examples	Removed Examples/TranSiesta directory, fi...	3 years ago
Obj	Merge from 4.1: IBM fixes; experimental ma...	4 months ago
Pseudo	Prepare GPL release	4 years ago
Src	maint: upgraded lapack for missing routines	4 days ago
Tests	Added h2o-shift-COP test	2 months ago
Tutorials	Revise mentions to now-standalone ATOM ...	4 years ago
Util	Merge branch 'rel-4.1'	1 month ago

<https://gitlab.com/siesta-project/siesta>

SIESTA COMMUNITY

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Name	Last commit	Last update
.gitlab	[admin]: Add BugReport and Suggestion is...	2 months ago
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<https://gitlab.com/siesta-project/siesta>



Wiki

User documentation

- [Overview of user documentation](#) ← SIESTA manual & tutorials
- [Guide to Siesta versions](#) ← Information on stable, beta-release & development branches

Developer documentation

- [Getting Started with Git and Gitlab](#)
- [Contributing to SIESTA](#)
- [Migration from Launchpad to Gitlab](#)

<https://gitlab.com/siesta-project/siesta/-/wikis/home>

SIESTA COMMUNITY



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Other Relevant Topics

← *building Siesta*
running with GPUs
using PSML pseudopotentials
using Lua

<https://gitlab.com/siesta-project/siesta/-/wikis/home>

SIESTA COMMUNITY



Forum:

☐ Summarizes the most relevant Q&A from SIESTA Mailing List
https://departments.icmab.es/leem/SIESTA_MATERIAL/Docs/list.html

☐ Topics are classified in Categories

<https://forum.simuneatomistics.com/>

22/09/20

The screenshot shows the SIESTA forum interface. At the top, there are logos for SIMUNE and siesta, a 'Log In' button, and navigation icons. Below the header, there are filters for 'all categories', 'Latest', 'Top', and 'Categories'. The main content is divided into two columns: 'Category' and 'Latest'.

Category

Category	Topics
SIESTA - Installation Questi... Topics included in this category should be related to SIESTA installation and compilation. ■ Compilation ■ Libraries ■ Download ■ Performance	13
SIESTA - Technical Feature... Please check whether the answer to your question is given in the SIESTA manual or has been discussed in this forum previously!	7
Pseudopotentials and Basi... A proper choice of pseudopotential and basis set is of fundamental importance while performing calculations. This category is designed to shed light on this topic. ■ Basis Set ■ Pseudo	7
Convergence Before passing to do calculations for production it is important to set up properly the SIESTA parameters. Depending on the simulation you want to perform you may want to adjust different kind of variables and parameters. This category is about which are the parameters interest and how to convergenc... ■ k-points ■ Real Space Box ■ SCF	8

Latest

S Optical properties by siesta ■ Physics Questions and Solutions	2	Aug 7
D How to calculate PDOS at a vacuum on top of a slab ■ Physics Questions and Solutions pdos	1	Jun 19
N Electronic Projected Density of States ■ DOS & PDOS pdos	2	Jun 10
E Calculate the BSSE correction in the van der Waals funcional	0	Jun 9
E Stress tensor ■ Material Properties stress	5	Jun 1
V Makov Payne correction	2	May 23
P Wave function coefficients in a calculation including spin-orbit ■ SIESTA - Technical Features an...	2	May 6
7 Compilation with OpenMPI	1	

16

SIMUNE ACTIVITIES

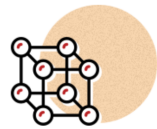


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Material Design



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SIMUNE ACTIVITIES

Automatization/Installation Tools:

➤ Binaries

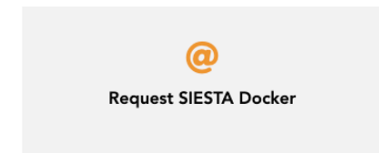
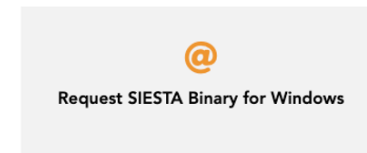
- Compilation/generation of SIESTA binary for Unix system (MacOS, any Linux distribution including HPC architectures)
- Compilation/generation of SIESTA binary for Windows 10

➤ Docker

- Deployment of SIESTA **Docker** images



Accessible from: <https://www.simuneatomistics.com/downloads/>



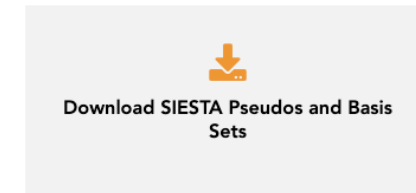
SIMUNE ACTIVITIES

Pseudopotential (psf) & Basis Sets:

1 H Hydrogen 1.008 0.506																	2 He Helium 4.0003 0.008															
3 Li Lithium 6.941 2.764	4 Be Beryllium 9.012 0.841																	5 B Boron 10.811 2.407	6 C Carbon 12.011 1.686	7 N Nitrogen 14.007 16.880	8 O Oxygen 15.999 8.502	9 F Fluorine 18.998 0.328	10 Ne Neon 10.180 0.026									
11 Na Sodium 22.990 1.696	12 Mg Magnesium 24.305 7.866																	13 Al Aluminum 26.982 0.699	14 Si Silicon 28.086 0.938	15 P Phosphorus 30.974 3.434	16 S Sulfur 32.066 4.284	17 Cl Chlorine 35.453 9.437	18 Ar Argon 39.948 0.928									
19 K Potassium 39.098 0	20 Ca Calcium 40.078 0	21 Sc Scandium 44.956 0	22 Ti Titanium 74.88 0	23 V Vanadium 50.942 0	24 Cr Chromium 51.996 0	25 Mn Manganese 55.845 0	26 Fe Iron 58.933 0	27 Co Cobalt 58.693 0	28 Ni Nickel 63.546 0	29 Cu Copper 65.38 0	30 Zn Zinc 69.723 0	31 Ga Gallium 72.631 0	32 Ge Germanium 74.922 0	33 As Arsenic 78.971 0	34 Se Selenium 79.971 0	35 Br Bromine 84.798 0	36 Kr Krypton 0															
37 Rb Rubidium 84.468 0	38 Sr Strontium 87.62 0	39 Y Yttrium 88.906 0	40 Zr Zirconium 91.224 0	41 Nb Niobium 92.906 0	42 Mo Molybdenum 95.95 0	43 Tc Technetium 98.907 0	44 Ru Ruthenium 101.07 0	45 Rh Rhodium 102.906 0	46 Pd Palladium 106.42 0	47 Ag Silver 107.868 0	48 Cd Cadmium 112.414 0	49 In Indium 114.818 0	50 Sn Tin 118.711 0	51 Sb Antimony 121.760 0	52 Te Tellurium 127.6 0	53 I Iodine 126.904 0	54 Xe Xenon 131.29 0															
55 Cs Cesium 132.905 0	56 Ba Barium 137.328 0																	72 Hf Hafnium 178.49 0	73 Ta Tantalum 180.948 0	74 W Tungsten 183.84 0	75 Re Rhenium 186.207 0	76 Os Osmium 190.23 0	77 Ir Iridium 192.217 0	78 Pt Platinum 195.085 0	79 Au Gold 196.967 0	80 Hg Mercury 200.592 0	81 Tl Thallium 204.383 0	82 Pb Lead 207.2 0	83 Bi Bismuth 208.980 0	84 Po Polonium [208.982] 0	85 At Astatine 209.987 0	86 Rn Radon 222.018 0
87 Fr Francium 223.020 0	88 Ra Radium 226.025 0	104 Rf Rutherfordium [261] 0	105 Db Dubnium [262] 0	106 Sg Seaborgium [266] 0	107 Bh Bohrium [264] 0	108 Hs Hassium [269] 0	109 Mt Meitnerium [268] 0	110 Ds Darmstadtium [269] 0	111 Rg Roentgenium [272] 0	112 Cn Copernicium [277] 0	113 Uut Ununtrium [289] 0	114 Fl Flerovium [289] 0	115 Uup Ununpentium [289] 0	116 Lv Livermorium [293] 0	117 Uus Ununseptium [293] 0	118 Uuo Ununoctium [293] 0																

Accessible from:

<https://www.simuneatomistics.com/downloads/>



For PSML Pseudopotentials: <http://www.pseudo-dojo.org/>

SIMUNE ACTIVITIES

Graphical User Interface:

- Integration of open-source codes
- User-friendly
- Customer support
- Multiplatform



REQUEST ASAP TRIAL VERSION

<https://www.simuneatomistics.com/services-products/asap-software/>

ASAP 20.03

Next Release: 20.10

ASAP developers: J. Alberdi, J. Albizuri, P. Koval, A. Larsen, F. Marchesin Y. Pouillon

SIMUNE ACTIVITIES



ASAP Main Window

Atoms	Label	Edit	Actions	Status
	CH3Cl CH3Cl; finite	Geom. opt Parameters SIESTA_4.0	Run Analyse	Completed
	NEB-Ag-difusion AgAu36; surface	NEB workflow Parameters emt	Run Analyse	New
	Pd111 Pd36; surface	Geom. opt Parameters SIESTA_4.0	Run Analyse	Completed
	H2O2 H2O2; finite	Single point Parameters SIESTA_4.0	Run Analyse	Completed
	Ag-bulk Ag; bulk	Phonons Parameters emt	Run Analyse	Completed

The Atomic Structure Builder

Create solid

Select element from Periodic table...

Co | Update lattice constant | hcp

Primitive Orthorhombic Cubic

Chemical formula of the unit cell Co2

Lattice constant (Å) 2,510000 1,622000

Unit cell:
2.5100 0.0000 0.0000
-1.2550 2.1737 0.0000
0.0000 0.0000 4.0712

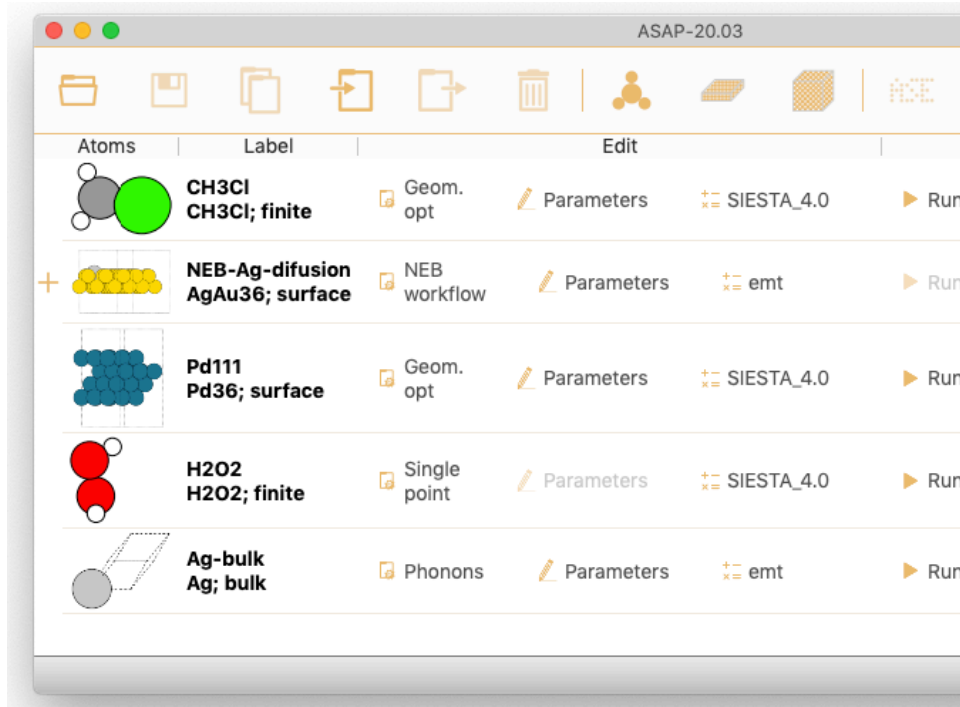
Cancel OK



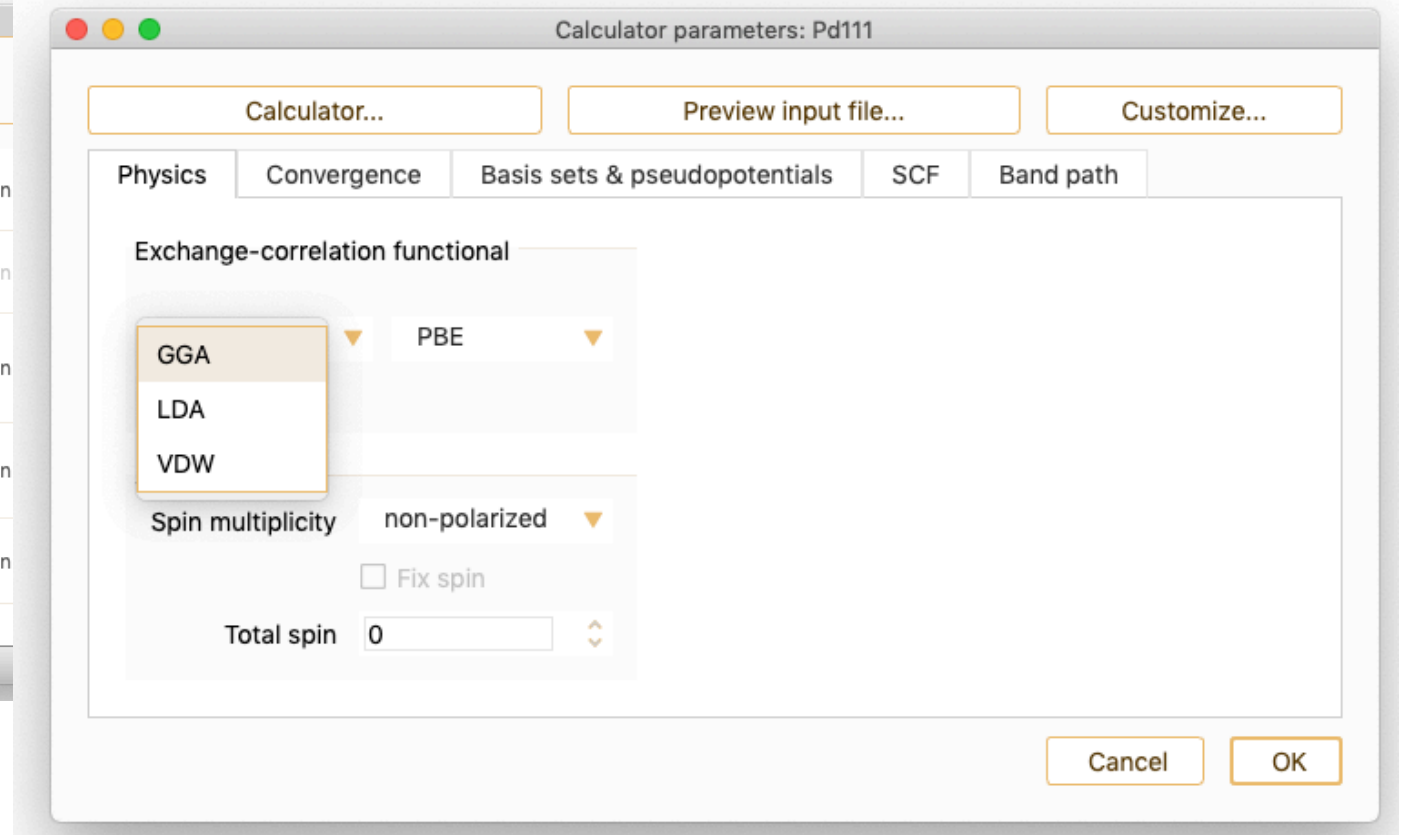
SIMUNE ACTIVITIES



ASAP Main Window



The SIESTA Calculator



SIMUNE ACTIVITIES



ASAP Main Window

Atoms	Label	Edit			
	CH3Cl CH3Cl; finite	Geom. opt	Parameters	SIESTA_4.0	▶ Run
	NEB-Ag-difusion AgAu36; surface	NEB workflow	Parameters	emt	▶ Run
	Pd111 Pd36; surface	Geom. opt	Parameters	SIESTA_4.0	▶ Run
	H2O2 H2O2; finite	Single point	Parameters	SIESTA_4.0	▶ Run
	Ag-bulk Ag; bulk	Phonons	Parameters	emt	▶ Run

Calculator

Physics Converge

Exchange-correlation

- GGA
- LDA
- VDW

Spin multiplicity

Total spin

Customize the input file

Find:

SystemName siesta
SystemLabel siesta

DM.MixingWeight 0.1
DM.NumberPulay 3
DM.UseSaveDM False
MaxSCFIterations 1000
PAO.BasisType split
SCFMustConverge True

Spin non-polarized
XC.functional GGA
XC.authors PBE

MeshCutoff 2721.1386024367243 eV
PAO.EnergyShift 0.1 eV

NumberOfSpecies 1
NumberOfAtoms 36
%block ChemicalSpecieslabel
1 46 Pd.gga.pbe.1
%endblock ChemicalSpecieslabel

%block PAO.BasisSizes
Pd.gga.pbe.1 SZP
%endblock PAO.BasisSizes

LatticeConstant 1.0 Ang
%block LatticeVectors
8.251936136447011 0.0000000000000000
0.0000000000000000
4.125968068223505 7.146386324569923
0.0000000000000000
0.0000000000000000 0.0000000000000000
16.737677641442932
%endblock LatticeVectors

Restore from dialog Interpret Save to dialog

OK

SIMUNE ACTIVITIES



ASAP Main Window

Atoms	Label	Edit	Actions	Status
	CH3Cl CH3Cl; finite	Geom. opt Parameters	SIESTA_4.0 Run Analyse	Completed
	NEB-Ag-difusion AgAu36; surface	NEB workflow Parameters	emt Run Analyse	New
	Pd111 Pd36; surface	Geom. opt Parameters	SIESTA_4.0 Run Analyse	Completed
	H2O2 H2O2; finite	Single point Parameters	SIESTA_4.0 Run Analyse	Completed
	Ag-bulk Ag; bulk	Phonons Parameters	emt Run Analyse	Completed

Analysis Widget

Analyse: Pd111

Atoms/Calculator/Project

siesta™

Energy series

Single-particle energies

Band structure

DOS

Show input...

Show output...

Energy

Reaction coordinate diagram showing energy E vs reaction coordinate R with R_{equ} marked.

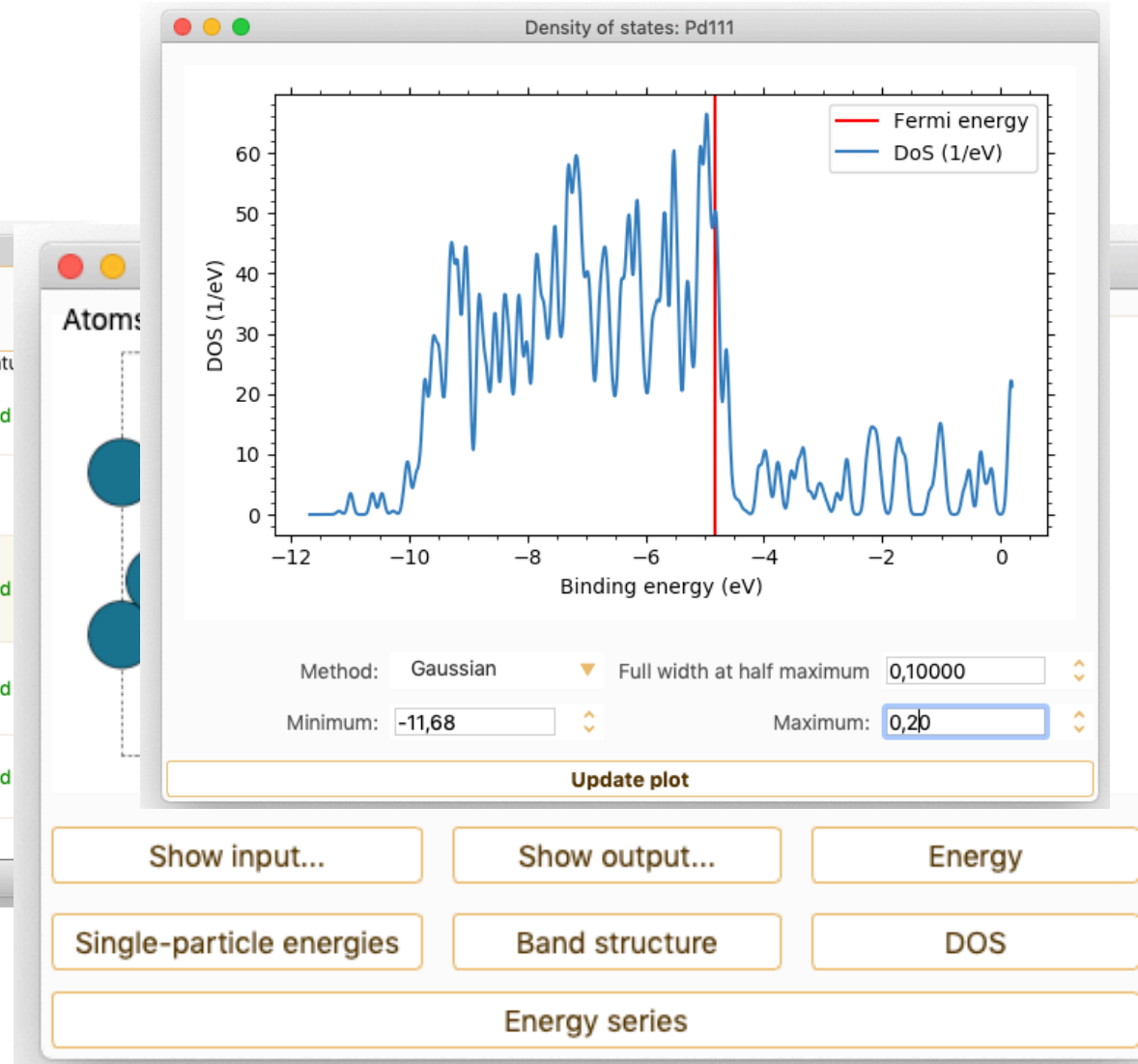
SIMUNE ACTIVITIES



ASAP Main Window

ASAP-20.03

Atoms	Label	Edit	Actions	Status
	CH3Cl CH3Cl; finite	Geom. opt Parameters SIESTA_4.0	Run Analyse	Completed
	NEB-Ag-difusion AgAu36; surface	NEB workflow Parameters emt	Run Analyse	New
	Pd111 Pd36; surface	Geom. opt Parameters SIESTA_4.0	Run Analyse	Completed
	H2O2 H2O2; finite	Single point Parameters SIESTA_4.0	Run Analyse	Completed
	Ag-bulk Ag; bulk	Phonons Parameters emt	Run Analyse	Completed





DRIVING THE EXASCALE TRANSITION

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 [@max_center2](https://twitter.com/max_center2)

 <http://www.max-centre.eu/>

THANKS