Webinar Questions

N°	Question	Answer
1	Sir, i want to learn siesta from basic, from where i can learn?	You can find manuals, tutorrials, a key publications reference list and the mailing list in this web page: https://departments.icmab.es/leem/siesta/Documentation/index.html
2	Please, can we run SIESTA on Windows? How?	We offer SIESTA docker and SIESTA Binary for Windows https://www.simuneatomistics.com/downloads/
3	Greetings Sir, I'm using ubuntu 19.10 and 20.04 on my systems. due to non-availability of BLAS library on these versions of ubuntu I'm unable to complete parallel installation of SIESTA on my system. If I can get any help regarding this.	Please, see the info in the last talk in this webinar by Mónica García, about user support channels.
4	I need a SIESTA version that uses hybrid functionals	Answer 1: Work is currently being done on this. If you follow the mailing list we will announce when such a version will be available. Answer 2: SIESTA with hybrids is still not in the public distribution. It will be soon. Please stay tuned, or ask Prof. Javier Junquera (javier.junquera@unican.es) for an alpha tester version.
5	Is force available for TDDFT calculations?	Yes, the forces are routinely calculated, as well as the stress tensor
6	I know somehow about siesta like DOS and Bandplot etc., can anybody help me for further, i will be very thankful for this, please guide me.	Here you can find tutorial material from Siesta schools. https://gitlab.com/siesta-project/siesta/-/wikis/Overview-of-user-documentation
7	Hello. For a given fixed amount of money. For SIESTA, is it better to have more CPU or less CPU+GPU is faster?	It really depends on your usage pattern.
8	How we can reach the PPs? Are the PPs are generated bu the users?	Pseudos have to be checked (and can be generated) by users. But SIESTA can use the pseudopotentials tabulated in the pseudo-dojo web site (with the very good pseudos of Hamann). Using the PSML format, Siesta can read and use them.

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9	Greetings sir, what GPU architectures does siesta support?	Currently Siesta supports the GPU's that ELPA supports. So as soon as ELPA has kernels for other GPU's, Siesta will immediately be able to use those. Additionally, if ELSI adds GPU support, Siesta will also immediately be able to use those architectures. Bottom line, Siesta has GPU support through 3rd party libraries and specific architecture support comes from them.
10	Are you planning to create a database of tested pseudopotentials distributed with the code (like, for instance, in VASP)?	Pseudos have to be checked (and can be generated) by users. But SIESTA can use the pseudopotentials tabulated in the pseudo-dojo web site (with the very good pseudos of Hamann). Using the PSML format, Siesta can read and use them.
11	Can we perform GW calculations in the updated version of SIESTA?	Not within SIESTA, but there is a post-processing program doing it, by Peter Koval and Daniel Sanchez-Portal, which is being bundled with Siesta by Simune.
12	Quick question about (PEXSI) talk, what are the main limitations behind such method?	The system needs to be large enough for the method to be past the cross-over point. Plus, you do not get eigenstates, but the density-matrix directly.
13	Hello, can we apply gate voltage in TransSiesta?	Yes, Siesta+TranSiesta allows two ways of adding gates: 1. One can add charged gates which implicitly calculates the potential response to the charges, for planar gates this is the same as a capacitor setup. 2. One can add user-defined Hartree potentials which mimics gates but these requires more specialized knowledge of the actual Hartree since they are not boundary conditions in the Poisson equation. In my talk I will present the charged gate (next)
14	If one uses pseudos in PSML format, do you need to rely on automatic generation of basis set or it must be done by user?	It is always better to have basis functions adapted to your pseudo. You can therefore define finite support confinement parameters etc independent of the pseudo, but then let siesta generate the basis function with those parameters for the actual pseudo being used.
15	Do you have any plan to include Machine Learning in the future SIESTA release?	Machine learning couldbe used for many things, but the main results of the siesta code are from first principles, and therefore, we do noty plan to use machine learning for the results of calculations (that would fit better with 2nd principles methods). SIESTA could be used as source of information for machine learning.

N°	Question	Answer
16	Hi! Thank you for the seminar! Remembering the difficulties, I had compiling SIESTA at the university cluster, I would like to ask -- do you plan to ship pre-compiled Linux binaries (as Gaussian or Turbomole do)?	This is certainly an issue for us too. We are working on ways to ease the installation.
17	I am wondering which version of SIESTA I should use as an end user. There are v4.1-b4, v4.0.2, Max 1.0.1 versions. All of these releases are quite old. There are various bug fixed on the updated channel of rel4.1, max versions on gitlab. If you can comment something about it, then it will be very helpful.	Answer 1: We will release a stable version of 4.1 soon, and then that will be what we recommend users. The MaX releases are connected with objectives of the MaX project. Currently, the 4.0.2 is the recommended release of Siesta due to its stability. Answer 2: If you can compile yourself, you are better off using the tip of the branches. The MaX version is actually quite recent, showcasing the latest bleeding-edge developments. Please see the Wiki.
18	Is it fine to have unequal layers on L & R side? on slide 8/9 here 5L on L side and 4L on R side!	Answer 1: TranSiesta allows asymmetric electrodes if so desired, so no problem. Answer 2: If you mean that the layers between the scattering region and the actual electrodes are different. There is no requirement of the number of layers between the two. In this case it was because of the stacking sequence.
19	I was using siesta version 4.0 b2 for one my project which is kind of not completed yet should I shift all my calculations to siesta 4.0.2?	Watch the webinar video for the live answer.
20	Also, please suggest a easy to use and open source visualizer in order to create/edit the geometry hence finally creating fdf file?	You will see more in the last talk in the webinar
21	I myself benefitted very much from the speed of doing MD simulations of water in between 2D materials in SIESTA. Also the possibility of making your own constraints in constr.f is just amazing! (for me it was a force dragging water molecules along CNTs) So I am very happy to hear that you include QM/MM functionality. Based on a quick scan of the reference paper I see that Amber forcefield is (will be?) implemented directly in SIESTA code. Are there plans to allow coupling to popular MD soft, like Gromacs or Amber?	Yes, AMBER is implemented within our QM/MM module. We do not have specific plans to link to MD software.

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22	I guess what pinned me was different number of layers in the buffer region. (electrodes were same)	Yes, you can use different number of layers, but you always have to check that the electrodes are thick enough to screen the effect of the contact (which is certainly not the case in the cartoons I showed).
23	Can the capacitance of the system be calculated directly, in the out, put file like the current in transiesta?	Not directly (it is not an output of the code), but can be computed indirectly from the quantities computed with TranSIESTA. It would involve integrating the charge transfered, which can be easily done with the utilities provided with SIESTA
24	Do transiesta calculations take too much time? Approximately? I know it depends on the system, maybe you can give an info.	The cost with the current version of TranSIESTA is not very much larger than the one of a standard SIESTA run of the same system size. In my experience, it can be a factor of 5, at most.
25	Dear Sir/Madam, I was using 4.0 b2 version for my old project which involves lots of calculations. As per the discussion in this webinar, I am kind of getting confused whether I recalculate all my old calculations with 4.0.2 version or not? As it will be really difficult and time consuming for me to do so. Kindly advise me. Thank You	As long as you have done a good calculation, you should not need to repeat it. Newer versions might offer new features or more performance, but unless you have been exposed to a bug, you should be fine. You might want to check a few calculations only.
26	Can the new version of Siesta take into account the crystal symmetry?	No. The dealing with symmetries in siesta is quite limited. It is relatively low in the priority list since the benefits of symmetry for large systems (especially moving) is quite limited. But there are tools that can be used for symmetry pre- and post-processing.
27	Is it possible to have collaboration with the presenters?	The presenters are science researchers. Collaborations work as usual in research. If there is interest on both sides.
28	Can TranSiesta consider tunneling current and spin polarized current?	Yes. For tunneling you need to be careful of the basis set
29	I don't quite understand what is the main difference between supercell and RSSE? Is there a way to recognize when to use RSSE?	In the supercell you have transverse periodicity, while in RSSE you don't have this. So generally, if you only have a single junction RSSE would be the most correct way to do it. However, it all depends on what you want to look into. If you correctly separate the images and they have a weak coupling, then you may rely on the supercell approach. However, in particular 3-terminal calculations with 2D materials the RSSE may provide much more reliable results.

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30	Is there any tutorial session today?	No, this is only a webinar. We are organizing both a SIESTA School and a TranSIESTA workshop in the first half of 2021. Stay tuned in the MaX and SIESTA web pages with the announcements.
31	How can I get a training period to master SIESTA in your Lab?	Given the limitations due to COVID-19, this will not be possible in the near future. Stay tuned for announcements of SIESTA and TranSIESTA schools in the next few months, through the MaX and SIESTA web pages.
32	I would like to thank everyone for this wonderful webinar. Could you email the videos link (for rewatch) or upload to youtube? Many thanks.	Watch the webinar video for the live answer.
33	Sir, can we do phonon calculations using siesta code? How accurate are the results w.r.t. other softwares?	Answer 1: There is the possibility of doing it using finite differences. Doing it via DFPT is quite recent, coming up. Answer 2: Yes, you have utilities that allow you to compute phonons within the SIESTA distribution package. The accuracy depends critically on the numerical parameters of your calculation, like the basis set and the spacing of the real space discretization, but can be as accurate as PW results.
34	How can we use HSE06 exchange- Hybrid functional in SIESTA?	Watch the webinar video for the live answer. You can contact SIESTA team directly.
35	Please suggest open source visualizer best suited for Siesta.	That depends on what you want to visualize, for atoms, use molden, jmol, ase or anything. For grids, you can use vmd and xcrysden.
36	Is Simune free?	Watch the webinar video for the live answer.
37	Thanks for nice presentations, If we can find reliable full relativistic pseudo files for transition metals to support SOC splitting?	You can try the pseudo-dojo database. You should download the PSML format pseudos.
38	There will be an academic version of ASAP?	Watch the webinar video for the live answer.
39	Sorry I would also like to know how can we use HSE06-Hybrid in Siesta?	You can contact SIESTA team directly.
40	How is SIESTA comparable with other LCAO codes (CONQUEST, OpenMX)?	Watch the webinar video for the live answer.
41	without using manual basis (orbital information), basis energyshift input, can we get publishable results?	You should always make sure that your basis set is appropriate.
42	Is it possible to do TDDFT calculations with hybrid functionals?	Watch the webinar video for the live answer.

N°	Question	Answer
43	Thank you for the presentation. I missed part of the talk and I hope my question is not redundant. Do you have a version taking into account an implicit solvent?	Not yet, but are working on integrating the Psolver poisson solver from BigDFT (see merge request in Gitlab)
44	Can I do quantum spin hall transport using the cross-shape schematic with four electrodes?	TranSiesta works for spin polarized calculations, but currently not non-collinear.
45	Is there any internship opportunity available at Max centre or Simune?	Watch the webinar video for the live answer.
46	What about Meta-GGA functionals (SCAN)?	They are underway….
47	Last time i asked about LDAor GGA +U it is still under test? Has the LDA+U been tested yet?	It is working in the more recent branches.
48	Can I plot spin pattern for rashba-effect from siesta post-processes? for non-collinear problems?	Check the Util directory in recent versions
49	I see, the output of psml siesta gives .psf files, can we use these .psf files for non-psml version of siesta ? (sorry if question is much crazy)	You can, with some caveats.
50	Thank you very much for an excellent seminar. I'd like to ask if NEB calculations are possible with non-collinear spin option.	Watch the webinar video for the live answer.

Thank you for joining the MaX webinar on “New developments in SIESTA for high-performance materials simulations”.

You may find the webinar video and slides here.