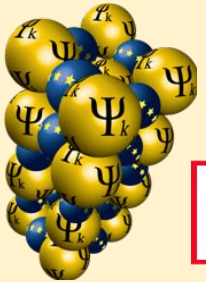
siesta Community Guidelines

Interacting with SIESTA beyond the command line



Centre Européen de Calcul Atomique et Moléculaire

Institut Català de Nanociència i Nanotecnologia

CSIC
Consejo Superior de Investigaciones Científicas

MAX DRIVING THE EXASCALE TRANSITION

Ministerio de Ciencia, Innovación y Universidades

Financiado por la Unión Europea NextGenerationEU

Plan de Recuperación, Transformación y Resiliencia

Agencia Estatal de Investigación

Where is 

?

Where is siesta ?

First, the webpage:

https://siesta-project.org/siesta/

- **Links to every other page that is SIESTA related.**
- Information on events organized by us and other SIESTA groups.
- Contact information.
- Info on basic gitlab interactions for starting developers.

Where is siesta ?

Tutorials and documentation:

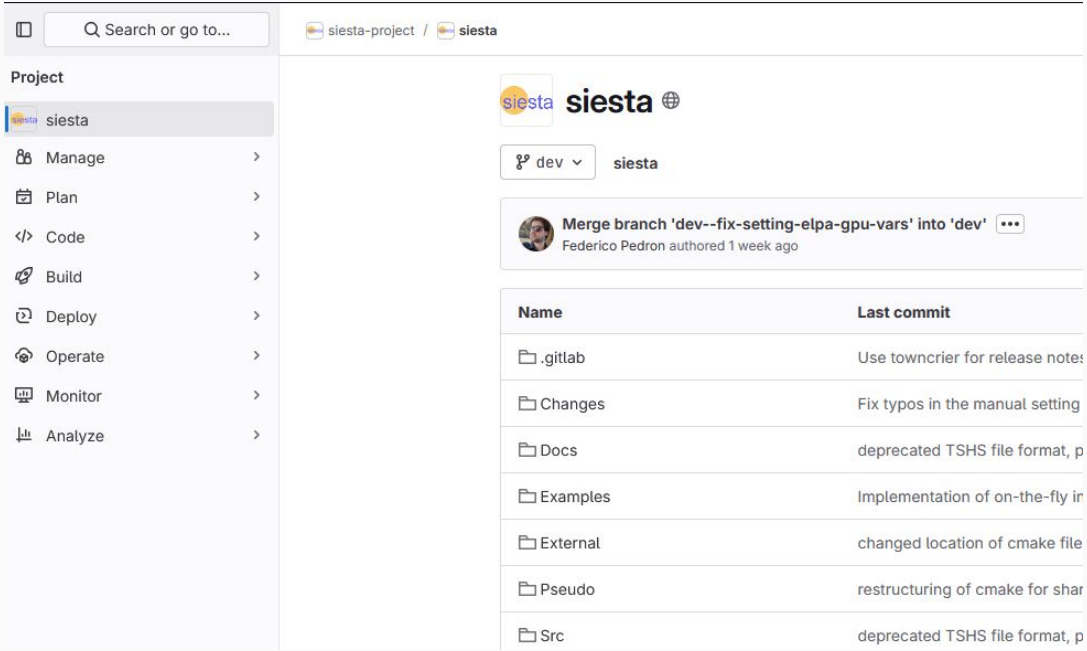
https://docs.siesta-project.org/projects/siesta/en/stable/

- Tutorials are in constant improvement.
- There is an online version of the manual!

Where is siesta ?

GitLab

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

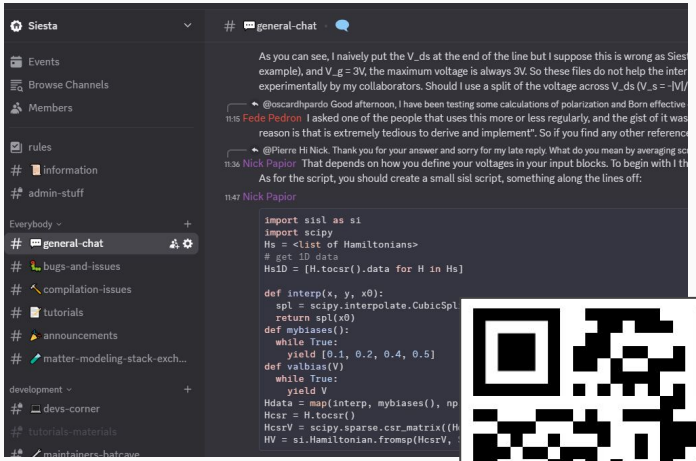


- Bug reports
- Code development

Where is siesta ?

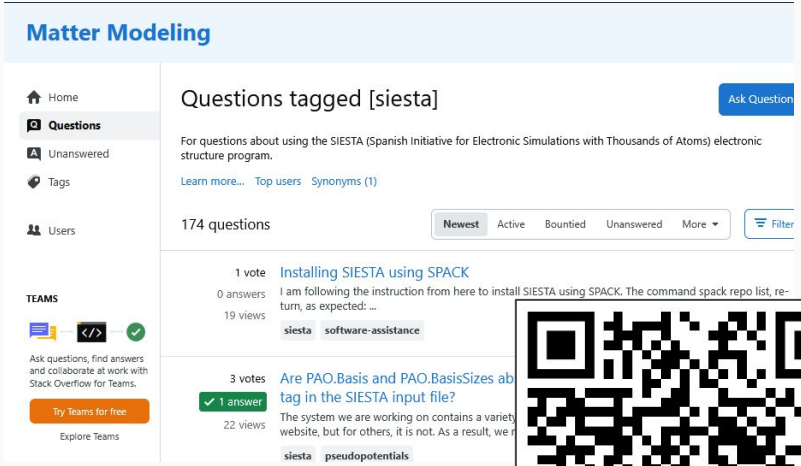
Discord

https://discord.gg/AqjX6aTNXR



Matter Modelling Stack Exchange

https://mattermodeling.stackexchange.com



Questions, bug reports, feature requests

Asking questions

Questions on general physics, discussions, literature:

- Ask them on Matter Modeling Stack Exchange! Replies will not be fast, but they're often thorough. Also, people from other codes also collaborate there.

Small questions on SIESTA usage, bugs or installation issues:

- Go to the discord! We usually reply fast, and do not leave questions out.

Asking questions

Please use **gitlab** for feature requests, thourough bug reports, or performance reports.

You can also do it via discord or email, but creating an issue in SIESTA's gitlab is the cleanest way (and saves us a lot of work). So if you're able, please do it!

Submitting code

Code submission

To interact with SIESTA at the software development level, **gitlab usage is mandatory**:

- we expect you to at least have a minimal knowledge on how git and gitlab works (**and if you don't, ask!** We're always ready to help).
- This is so we can keep proper records of who added which modification to the code.

Code submission

If you're working on a new development for SIESTA, please open an issue and/or MR in the main repo: this way *we get to know who is working on what*.

If your addition to SIESTA is large or complex (or very disrupting) please coordinate with maintainers before rushing headlong into an implementation.

As soon as you want to, *open a merge request* towards the main repo with your developments.

Code submission

For the code to be merged, we actually require few things:

- The code must be tested enough. The tests within SIESTA at least should work properly. If there's a new functionality, a new test for that functionality is also expected.
- The code must be well documented, and comply with a given coding style. People should not rely on the original developer to explain the code.
- A release notes file should be added under /Changes (see the readme at /Changes/README.md).
- Any new fdf options or run modes should be documented in the manual (under /Docs) in LaTeX format.

Code submission

Opening a Merge Request is **the first step**, it **does not mean your work is done**!

We might ask for:

- Specific tests for compatibility.
- Added documentation
- Consistency with other SIESTA internals or existing input options (if we already have *NumberOfAtoms*, avoid doing your own *TotalAtoms* input option).

Code submission

Are you bored, have some free time, and want to collaborate?

Check out the “needs-collaborator” milestone; it usually has features that we have been leaving out due to time.

https://gitlab.com/siesta-project/siesta/-/milestones/15#tab-issues