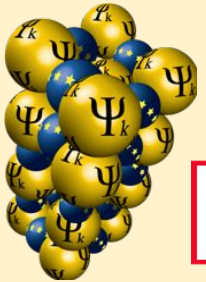
siesta™ Advanced Workshop

Concluding remarks?



cecam
Centre Européen de Calcul Atomique et Moléculaire

ICN2
Institut Català de Nanociència i Nanotecnologia

CSIC
Consejo Superior de Investigaciones Científicas

MAX
DRIVING THE EXASCALE TRANSITION

MINISTERIO DE CIENCIA, INNOVACIÓN Y UNIVERSIDADES

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Plan de Recuperación, Transformación y Resiliencia

AGENCIA ESTATAL DE INVESTIGACIÓN

A change in execution paradigm?

- An important portion of the tutorials was executed in notebooks and/or with conda installations.
- Is this only for teaching purposes? Or is this becoming the mainstream way to execute stuff?
- What about sisl? Does this replace our Utils?
- Does this turn things into a more “blackbox-y” approach?

Emergent technologies

- In which ways do we incorporate Machine Learning? What are the possibilities for large-scale workflows?
- Are there ways in which we can leverage “AI”? (other than the obvious)
- Are there lines where these technologies should **not** go? (do not yell at clouds, think)

Emergent technologies

- The best way to predict the future is to create it.
- The future comes, whether you like it or not.
- Do not fight the wave, ride it. Do not go against the flow, redirect it.

A call for community

A time of fragmentation

- Which pieces of software do you use for your calculations? How much do you have to learn about them?
- What do you use for scripting? Bash? Batch? Perl? Python?
- And plotting… gnuplot, matplotlib, different python packages… (note the appeal of python as a catch-all)
- How do you write your scientific communications? Word? Latex? Docs? Which plugins? Which platforms?

A time of fragmentation

- How do you interact with other people? Email (which account)? LinkedIn? Bluesky/Twitter? Discord?
- Do you *doomscroll* and not comment/post? Do you post and not read?
- Migrations due to *enshittification*. (Twitter, who's next?)
- No single person can be an expert in everything… and no longer a single person can know everything in a single area.

A call for community

- We cannot longer call each other at 3 am to finish a paper.
- We are a lot of people!
- There is a lot of thing to test, maintain, reproduce…

A call for community

- Answer other peoples' questions!
- Engage your own students!
- Report stuff!
- What can we do to get you do write documentation???

A call for community

- Keep sharing
- Keep discussing
- Keep learning!