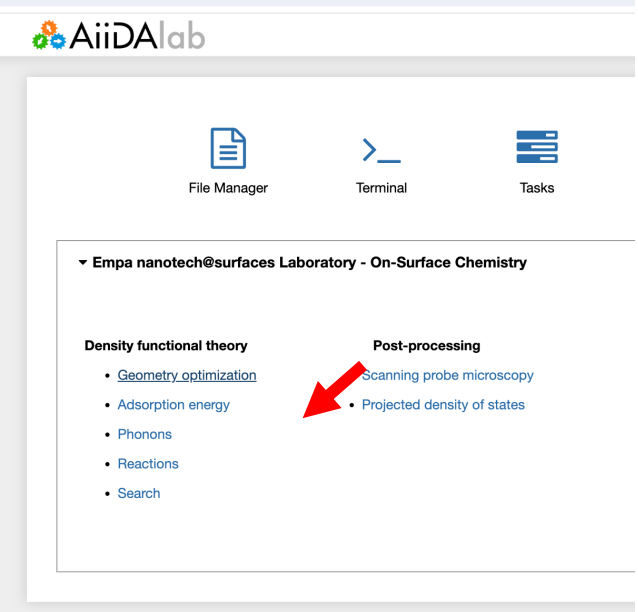
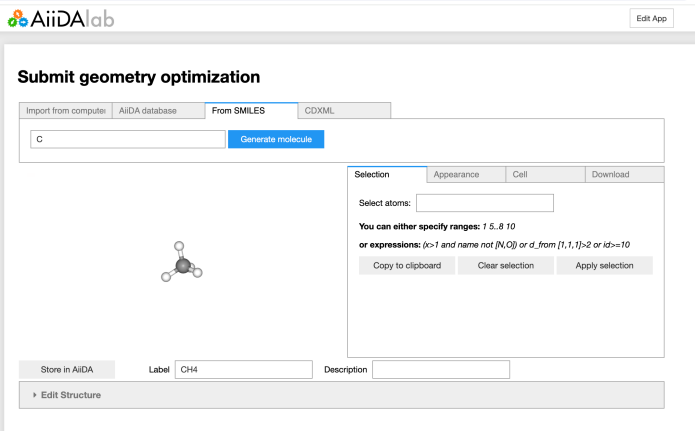
Setting up a «computer» on piz daint (CSCS Lugano)

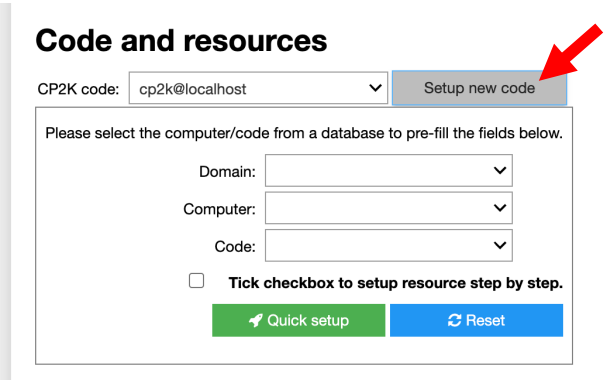
Start with clicking on “Submit geometry optimization”



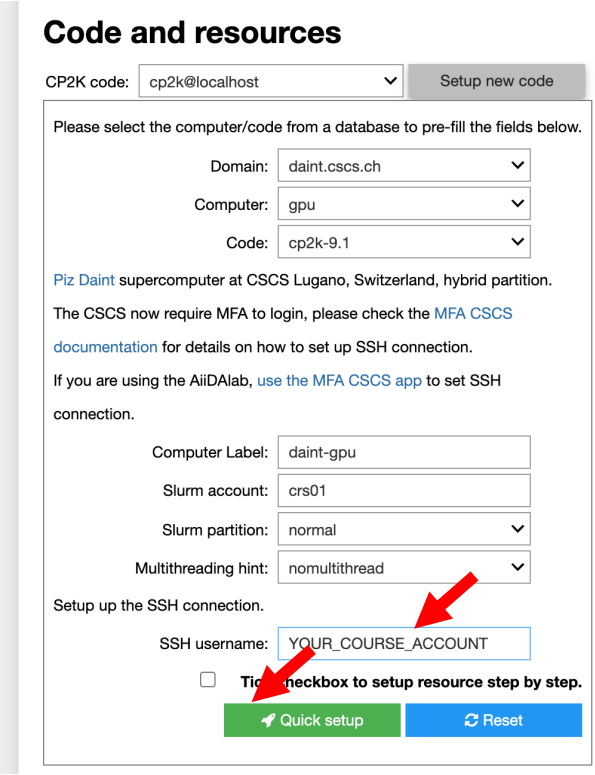
Insert any molecule (e.g. SMILES for methane)



Scroll down to “Code and resources”, hit “**setup new code**”



Give the following parameters (including the course account name you got per E-Mail, and hit “Quick Setup”



At this point, go to the “Exercise9” directory and give the command:

“./initialize_daint.sh”

This will copy the private key to your ~/.ssh directory .

The public key of your account courseXX (with XX=01—30) is already on the supercomputer.

Go to a terminal and give the command

- ssh daint.cscs.ch

if it connects to daint without password, **very good!** Hit “exit” and go back to your shell.

If not, give the command

- ssh-copy-id daint.cscs.ch

and give the password you got by email as many times as requested.

Then try

- ssh daint.cscs.ch

You will be requested the password, exit then daint and repeat until the password is not requested anymore.

The content of the file ~/.ssh/config is:

(base) jovyan@d633c698dc55:~$ more .ssh/config
Host daint.cscs.ch
User course18
Port 22
ProxyCommand ssh -q -Y course14@ela.cscs.ch netcat daint.cscs.ch 22
ServerAliveInterval 5

Now, when you want to start a geo opt on daint, select the corresponding computer/code as in the following figure: