Targeting Real chemical accuracy at the EXascale

Build-system Hackathon

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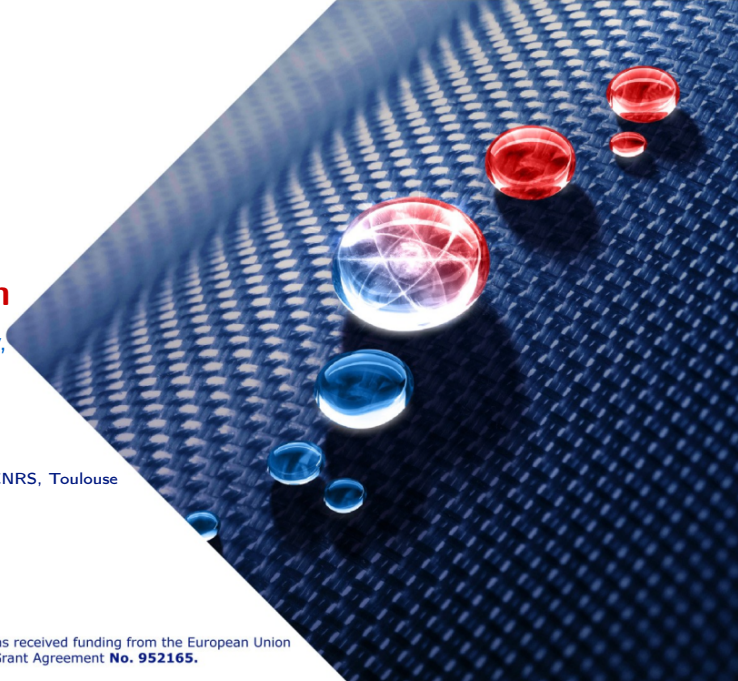

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Objective

- Understand how the CMake and GNU Autotools build systems work
- Improve the way you distribute your software

Why?

- When you can't use your own software on a new machine, you are frustated
- When users download your software and are not able to install it, they look for another one
- If they really need that software, they will you bother you asking for help
- Once set up, it will save you a lot of day in every day development

Important

We don't support the Windows OS in this hackathon.

Presentations

- Short intro to CMake (Radovan Bast) and Autotools (Christian Feld): you will start to decide which one you prefer using for your project.
- Longer tutorials on CMake (Radovan) and Autotools (Evgeny, Anthony) to confirm your choice and to start to diving into it.

Work on your own code

- Improve your Makefiles
- Introduce/improve your CMake/Autotools scripts
- Ask plenty questions to us or other participants
- During hands-on sessions, work as you prefer: take breaks when you want, etc. It is a moment where we are available for questions.

Helpers

- Anthony
- Evgeny
- Vijay
- Pablo
- Radovan

Zoom

- You will be separated in break-out rooms, one for each team.
- Those who are alone in their team can join in a common room

Slack

- The Zoom chat will be disabled.
- All written/chat communication should be done via Slack
- You can use Slack to communicate asynchronously with helpers that are not on Zoom

We expect you to

- Present your code and how it is installed. It should not be optimal, otherwise you would not be here! Don't be shy!
- Present to others in detail the progress you made for your code, sharing with others tips and tricks, useful links on the web etc
- *Code-swapping*: Take the code of other teams, try to install it on some of your machines and give some feedback

Note

Don't spend too much time preparing a nice presentation. You can improvise sharing your screen and showing things live.

Presentations

Now your software can build, how to go beyond:

- HPC Containers (Kai Löhnig)
- Guix-HPC (Ludovic Courtès)
- Conda (Leopold Talirz)
- Spack (Todd Gamblin)

Special Thanks

- European Commission (TREX Center of Excellence)
- EuroCC National Competence Center Sweden
- All the invited speakers: Christian Feld, Kai Löhnig, Ludovic Courtès, Radovan Bast, Todd Gamblin, Nico Mittenzwey, Leopold Talirz