

# exciting: porting a full all-electron full-potential DFT code to GPU

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What we wanted to do

# Main objectives in this Hackathon

- ▶ Enable the compilation with offloading to GPUs with Cray compilers.
- ▶ Port the complex loop that computes the expansion coefficients (currently implemented using OpenMP for CPU execution).

# What we achieved

# Outcomes from this Hackathon

Enable the compilation with offloading to GPUs with Cray compilers.

- ▶ The code now compiles and the data transfers are as expected (CCE 18.01, specifically OpenMP “has\_device\_addr”).
- ▶ We found a non-evident race condition in the CPU code and we solved it (use Cray sanitizer, compiler flag “-fsanitize=thread”).

Port the complex loop that computes the expansion coefficients (currently implemented using OpenMP for CPU execution).

- ▶ We refactored the loop to make it more suitable for the GPU, the porting is WIP.