

DIADEM (Material Acceleration Platforms) and NUMPEX (HPC) projects

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Abstract

In this talk, I will explain the objectives of the French national DIADEM project, which aims to accelerate the discovery of materials using artificial intelligence, with the implementation of a database and workflow infrastructure. I will then focus on the French national NUMPEX project, which aims to provide the software stack for the next French exascale computer.

Finally, I'll illustrate the contribution of these projects on a concrete case of workflow mixing simulations and data analysis from ESRF synchrotron X-rays studying chemical reactions catalyzed by the surface of specific materials.

For any question, please contact contact@emmc.eu

References

<https://www.pepr-diadem.fr/en/>.