DIADEM (Material Acceleration Platforms) and NUMPEX (HPC) projects: Illustrating the application of BigDFT to proteins

Luigi Genovese[1], Cinthya Herrera-Contreras[1], and Thierry Deutsch[1]

[1] UGA, CEA, Material Exploration, and Modelling (MEM), Grenoble

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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 will illustrate the contribution of these projects on a concrete case of DFT calculation workflows for proteins containing several tens of thousands of atoms, with a reduction in complexity to provide quantities of interest to biologists.

For any question, please contact contact@emmc.eu

References

[1] Saber, M., Kotan, H., Koch, C. C. & Scattergood, R. O. A predictive model for thermodynamic stability of grain size in nanocrystalline ternary alloys. Journal of Applied Physics 114, 103510 (2013).