

Community codes at the exascale for advanced materials

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Abstract

Data driven materials research and discovery will continue to leverage key advancements of first principles codes, combined with frontier HPC architectures. I will discuss success cases and current challenges from the perspective of the MaX European Centre of Excellence [1,2] and its open-source community codes, workflows and platforms.

References

- [1] www.max-centre.eu
- [2] <https://max-centre.eu/software/codes>