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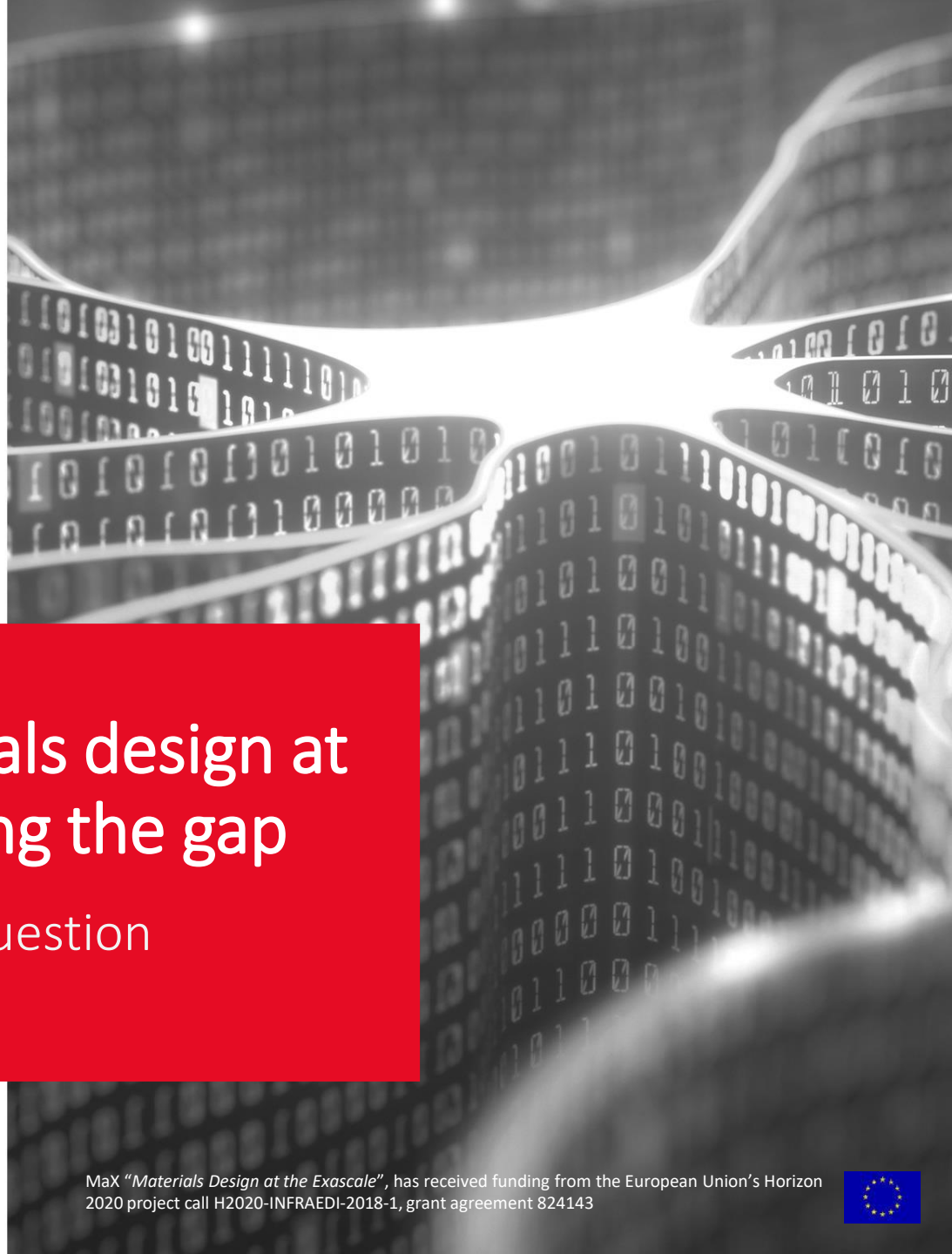
THE EXASCALE
TRANSITION



MaX Webinar
Industry and Materials design at the eXascale: bridging the gap

Answers to the Advance question

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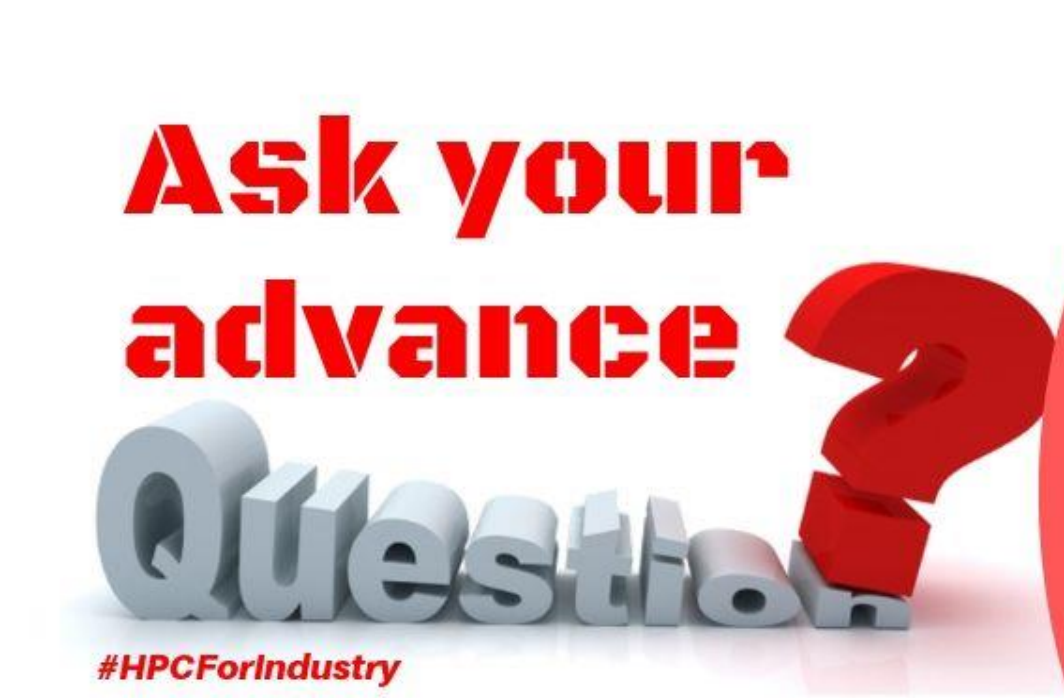
MaX Webinar: Answers to the Advance Questions



Thank you for sending your advance questions!
See you on the next MaX webinar.

MAX DRIVING THE EXASCALE TRANSITION

WEBINAR

Industry and Materials design at the eXascale: Bridging the gap

4th September, 2019, 10AM CEST

Watch the recorded webinar video

Q1: Question: How do MaX assets, uses cases, codes the materials cloud platform see to make a mark as part of the evolving European Open Science Cloud (EOSC)?

Answer by Giovanni Pizzi, EPFL

MaX has been interacting extensively with the EOSC to identify services to be added to the EOSC (see e.g. Giovanni Pizzi's participation to the EOSC-hub week in April 2019, discussing exactly this topic: https://www.eosc-hub.eu/events/eosc-hub-week-2019/programme/hpc-centres-excellence-eosc-arena).

Goals are discussed in the end of the presentation (available online)
In particular, here are the goals (some of them already reached since the presentation):

- Since June 2019, Materials Cloud is one of the communities of EUDAT's B2FIND, part of EOSC: http://b2find.eudat.eu/group/materialscloud
- Since July 2019, the Materials Cloud authentication is hooked to the "EUDAT's B2ACCESS" and "EGI Checkin" Authentication and Authorisation Infrastructures of EOSC
- Since August 2019, an open AiiDA lab demonstrator is running on the kubernetes cluster administered by CESNET of the EOSC-hub (see https://www.materialscloud.org/work/aiidalab)
- We are scheduling to register the AiiDA lab as one of the EOSC services after a beta testing phase, by the end of 2019
- We are scheduling to register the Materials Cloud Archive (by the end of 2019 - early 2020) as one of the EOSC services (after migrating the backend infrastructure from the current custom-developed one to CERN's invenio v3).

Q2: What is the strategy to adapt the flagship codes of MaX to the architectural features of the eXascale systems? And these codes will continue to run with reasonable performances also on small-sized systems?

Answer by Andrea Ferretti, CNR-Nano

A similar question has been addressed during the webinar, here I complement the answer. Yes, MaX flagship codes are meant to be used on both large and small size machines and this is going to stay. Moreover, some usage models of large scale architectures, eg the high throughput computing (HTC) model, put emphasis on the intra-node or few-node performance of each calculation. Thousands or tens of thousands of these small calculations are then run in bundles in order to perform a computational screening of materials properties (thereby making a case for large computational facilities). HTC is one of the key usage models in materials science and intra-node performance is surely within the target of MaX.

Concerning strategies, we have interacted with HPC experts and computer engineers from HPC centres and identified some strategies to deal with HW evolution. Here HW-SW separation of concerns is a crucial aspect. The software developers (scientists) which implement new scientific features in the codes should be exposed at least to the SW parts that are HW specific, and vice-versa. Only separing concerns the development model can scale. Such approach is put in practice by encapsulating data and methods, restructuring the code architecture to expose a number of SW components with well defined APIs (to be designed) possibly hiding specific low level implementations. MaX has a critical mass larger than that of single research groups active in the development of one tool and can leverage this to make such a paradigm change.

Q3: I have a problem in understanding the origin of a failure in a specific industrial process. I think that simulations could help, but I am not familiar with specific methods/codes. Can I still get help from MaX ? Whom should I approach ?

Answer by Andrea Ferretti, CNR

Support and services are core activities within the mission of MaX. For help-desk support (most suited for well-defined problems which can be handled technically over an email exchange) we have setup a user unique entry point via support@max-centre.eu . Here both technology/HPC issues and electronic structure/materials science problems can be addressed by MaX experts. For problems that require more interaction, as seems to be the case here, we also have a service of consultancy (for pay) which can be activated upon contact with MaX. The same entry point support@max-centre.eu can be used.

Q4: We typically use vibrational spectroscopy (Raman) to check the local strain conditions of materials/interfaces. Can I get support from simulations to interpret the spectra? This would be useful in cases where the materials/interfaces are not well known/characterized experimentally.

Answer by Pablo Ordejon, ICN2

Yes, several of the MaX codes provide the calculation of Raman spectra of materials. Some of the research groups involved in MaX are pioneers in the development and use of tools for the analysis of vibrational modes in materials, and have a long expertise in this matter. Support can be provided from MaX, on a specific basis that could be discussed with the particular groups.

Q5: Can the codes supported by MaX run on a small cluster with GPUs

Answer by Andrea Ferretti, CNR-Nano

All MaX codes that have been ported on heterogeneous systems accelerated with GPUs would do, independently on the size of the machine. So far most of MaX codes have already released such support (see eg Quantum ESPRESSO, BigDFT, CP2K, Sirius) or have beta versions ready to be released soon.

Thank you for joining!

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