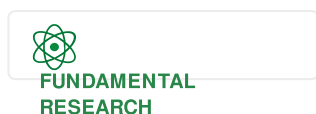


 Content archived on 2022-07-06

Managing, simplifying and disseminating High-Throughput computational materials science with AiiDA, AiiDA lab, and the Materials Cloud Archive

The second webinar of a series presenting the most recent developments of the MaX flagship codes entitled "Managing, simplifying and disseminating High-Throughput computational materials science with AiiDA, AiiDA lab, and the Materials Cloud Archive" will be held on 27 May 2020 at 3 PM CEST.




 27 May 2020 - 27 May 2020


 Online, Italy



Description

The available computational power has steadily increased over the past decades and continues to do so, with upcoming superclusters going towards a performance on the scale of Exaflops/s. These advances present great new opportunities for computational science but also pose new challenges with respect to how to automate the resources and manage the data that will be produced.

We will give a short introduction to [AiiDA](#) , a tool that is designed to help its users leverage high-performance

computing resources to automate workflows of HPC codes, such as those developed by [MaX](#) , run on those systems and manage the data that they produce. We will detail especially how the recent release AiiDA 1.0 comes with many performance improvements in the workflow engine and database in order to support high-throughput computational loads and the various mechanisms that allow its users to make

optimal use of current and future powerful HPC resources. After that, we will exhibit AiiDA lab, a GUI solution on the cloud that makes running these workflows and analyzing the results easy and intuitive, even for non-experts. Finally, we will present the renewed Archive of the Materials Cloud that serves as a dissemination platform that can be used to very easily publish data generated through AiiDA.

In this webinar, we will show how the MaX flagship code AiiDA supports its users to manage their computational workflows and the data that is produced. As opposed to all other flagship codes, AiiDA itself is not a simulation software, but instead is a workflow and data management tool. We will show how it can be used to automate workflows that directly employ the other MaX flagship codes, such as Quantum ESPRESSO, how AiiDA lab provides a user-friendly GUI to the workflows even for non-experts, and how the resulting data can easily be published through the Materials Cloud Archive.

REGISTER NOW! [↗](#)

Visit the [official webinar page](#) [↗](#) and see the exciting agenda prepared for its attendees.

MaX webinar series

This seminar is included in a series presenting the most recent developments of the MaX flagship codes. The next planned appointments are for [Yambo](#) [↗](#) (June 16) and [CP2K](#) [↗](#) (June 24). Stay tuned for the next announcements!

About MaX

MaX - Materials design at the Exascale has received funding from the European Union's Horizon 2020 under Grant Agreement n. 824143. Led by CNR (Italy), the MaX consortium partners includes SISSA (Italy), ICN2 (Spain), JUELICH (Germany), CEA (France), EPFL (Switzerland), Universiteit Gent (Belgium), CINECA (Italy), BSC (Spain), ETHZurich (Switzerland), E4 (Italy), ARM (United Kingdom), ICTP (Italy), Trust-IT (Italy).

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MaX



14 September 2023

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7 August 2019



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MaX European Centre of Excellence (CoE): Leading the path to materials design and beyond Exascale in Europe



29 June 2019

MAX DRIVING THE EXASCALE TRANSITION

MAX WEBINARS DATE: NOV 12 2020 TIME: 10.00 (CET)

The Flexibilities of Wavelets for Electronic Structure Calculations in Large Systems

SPEAKERS

Thierry Deutsch CEA	Laura Ratcliff Imperial College London	William Dawson RIKEN	Augustin Desgarnes CEA	Luigi Genovese CEA
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The Flexibilities of Wavelets for Electronic Structure Calculations in Large Systems

12 November 2020

Online, Italy

6 November 2020

MAX DRIVING THE EXASCALE TRANSITION

MAX WEBINARS DATE: OCT 14 2020 TIME: 11.00 (CET)

All-electron DFT using the **FLEUR** code

SPEAKERS FROM FZ-JUELICH

Gregor Michalczek	Uliana Alekseeva	Daniel Wortmann
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EVENT max-centre.eu

ARCHIVED

All-electron DFT using the FLEUR code

14 October 2020

Online, Italy



30 September 2020

MAX DRIVING THE EXASCALE TRANSITION

MAX WEBINARS DATE: SEP 22 2020 TIME: 15.00 (CEST)

New developments in **SIESTA** for high-performance materials simulations

SPEAKERS

Emilio Artacho Univ of Cambridge and Nanogune	Alberto Garcia ICMAB-CSIC	Pablo Ordejon ICMAB-CSIC	Nick Papadimitrakis DTU	Monica Garcia-Mota Simula
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EVENT max-centre.eu

ARCHIVED

New developments in SIESTA for high-performance materials simulations

22 September 2020

Online, Italy



10 September 2020




MAX WEBINARS

DATE JUN 24 2020 **TIME** 11.00 (CEST)

HPC libraries for **CP2K** and other electronic structure codes

SPEAKERS FROM CSCS

Anton Kozhevnikov	Shoshana Jakobovits	Simon Frasch	Marko Kabic
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EVENT

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ARCHIVED

HPC libraries for CP2K and other electronic structure codes

📅 24 June 2020

📍 Online, Italy



3 July 2020




MAX WEBINARS

DATE JUN 24 2020 **TIME** 11.00 (CEST)

HPC libraries for **CP2K** and other electronic structure codes

SPEAKERS FROM CSCS

Anton Kozhevnikov	Shoshana Jakobovits	Simon Frasch	Marko Kabic
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EVENT

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ARCHIVED

HPC libraries for CP2K and other electronic structure codes

📅 24 June 2020

📍 Online, Italy



19 June 2020




MAX WEBINARS

DATE JUN 16 2020 **TIME** 15.00 (CEST)

Quasiparticle Band Structures and Excitons in Novel Materials using the **Yambo Code**

SPEAKERS

Daniele Varsano CNR NANO	Andrea Ferretti CNR NANO	Andrea Marini CNR ISM	Myrta Grüning Queen's University Belfast	Maurizia Palumbo University of Rome Tor Vergata
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EVENT

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ARCHIVED

Quasiparticle Band Structures and Excitons in Novel Materials using the Yambo Code

📅 16 June 2020

📍 Online, Italy



5 June 2020




MAX WEBINARS

DATE MAY 13 2020 **TIME** 15.00 (CEST)

How to use **Quantum ESPRESSO** on new GPU based HPC systems

SPEAKERS

Fabio Affinito CINECA	Pietro Delugas SISSA	Pietro Bonfà Univ. Parma & CNR Nano
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EVENT

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ARCHIVED

How to use QUANTUM ESPRESSO on new GPU based HPC systems

📅 13 May 2020

📍 Pisa, Italy



27 April 2020

Last update: 15 May 2020

Permalink: <https://cordis.europa.eu/event/id/147912-managing-simplifying-and-disseminating-high-throughput-computational-materials-science-with-a>

European Union, 2025

