DRIVING
THE EXASCALE
TRANSITION

MaX Webinar: BigDFT

The Flexibilities of Wavelets for Electronic Structure Calculations in Large Systems

MaX "*Materials Design at the Exascale*", has received funding from the European Union's Horizon 2020 project call H2020-INFRAEDI-2018-1, grant agreement 824143

Welcome to the **last** MaX webinar !

We conclude the series
Of the presentation of the MaX
Flagship codes

7th event, series started May 13th

Go to
http://www.max-centre.eu/events/max-webinars
For the materials and recorded video (including this!)

TODAY

BigDFT code

A different formalism for
Electronic Structure Calculations

Plan of the Webinar

Structure of the presentation


T. Deutsch, L. Genovese
Basics of BigDFT Formalism
~30’ + Questions


L. Ratcliff, W. Dawson
Challenges in Large-Scale Calculations
~35’ + Questions

A. Degomme, L. Genovese
Software approach, HPC, Perspectives
~20’ + Final Questions Session

The objective of BigDFT project is to test and implement new ideas for DFT-based calculations. → Poll questions will be asked

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THANKS

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