

EMMI Workshop "Accurate relativistic treatment of multi-electron atoms
and applications to Super-Heavy elements"



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Integral and tensor interfaces and their use on supercomputers

Monday, 24 October 2022 15:00 (30 minutes)

For matrix operations It has become standard to interface code to the LAPACK and BLAS libraries and leave the optimization and compilation of these libraries to computer scientists and support staff at computing centers. We will give a short overview of available libraries for tensor operations and integral computation and want to start a discussion on their use and design. Additionally, we will discuss our experiences on supercomputers.

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