

Containerization in Modern Scientific Applications

Wednesday, October 24, 2018 11:15 AM (15 minutes)

Scientific algorithms for the solution of the correlated many-body problem and beyond are rapidly growing in complexity. This development shows also in their respective numerical implementations, leading to growing number of library dependencies, toolchain dependencies as well as inter-dependencies with other scientific applications. This often makes a proper setup on workstations, but in particular on high-performance cluster machines an ambitious and sometimes insurmountable task. In this presentation I will give an introduction into modern containerization tools, in particular Docker and Singularity, that are targeted to overcome these issues.

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Session Classification: Lightning Talks