



Contribution ID: 147

Type: **not specified**

Application of high-performance computing in battery development showcased for electrolyte filling

Monday, November 28, 2022 1:30 PM (30 minutes)

A workflow for battery performance optimization is presented that couples wetting and flow simulations based on pore network models (PNM) and the lattice Boltzmann method (LBM) with electrochemical simulations using the tool BEST. All software packages included show an appropriate scaling behavior on high-performance computing (HPC) clusters. Electrolyte filling of battery components is discussed as a showcase. This step is time-critical and therefore cost-intensive in battery manufacturing. A special focus is given to the unwanted side effect of gas entrapment encountered during the filling, which is also known to have a strong influence on the electrochemical performance of batteries.

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Session Classification: Poster session