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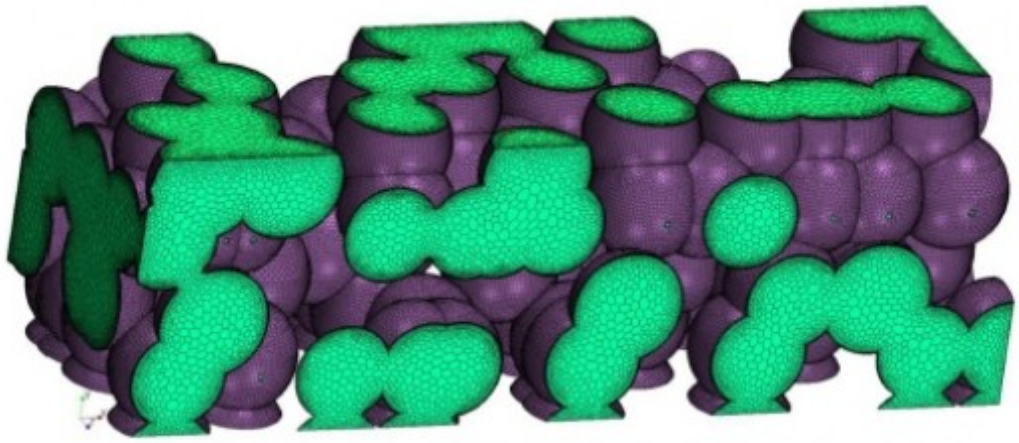
Geometry-Resolved Electro-Chemistry Model of Li-Ion Batteries



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Abstract:

The paper presents a simulation approach to Li-Ion batteries based on geometrically resolved electrodes. This means that solid particles and the space occupied by electrolyte are not overlapping but are represented by contiguous, arbitrarily shaped volumes. The solid-electrolyte interface is explicitly resolved and thus allows detailed modeling of electrochemical processes that are essential for studying performance of the battery cell. Finite volume method is used to solve the equations governing the mass and thermal energy conservation in solid and electrolyte, as well as the distribution of electric potential. The solution domain is discretized in contiguous control volumes of arbitrary polyhedral shape, with conformal interface between solid and fluid regions. Butler-Volmer equation is used to describe the kinetics of solidelectrolyte interface. For the time being, representative geometries of electrodes are manufactured using CAD-tools, but real geometries obtained using scanning methods will be used in future. One example application is presented and the results are compared to those obtained using a widely accepted one-dimensional method.

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