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An eXtended finite element method for the Nernst-Planck-Poisson equation

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Abstract: The Nernst-Planck-Poisson (NPP) set of equations is used to study the drifting mechanism in mixed ionic electronic conductors, commonly used in storage batteries. Depending on the size of the computational domain, the solution exhibits steep gradients near the boundaries, esp, in polycrystalline materials. As the grain boundary has different crystallographic orientations when compared to the bulk, to minimize the overall energy, charged defects redistribute between the grain boundary and the bulk grain. This redistribution introduces a steep gradient of ionic concentration and electric potential near the grain boundaries. Traditional finite element method, when employed requires extremely refined mesh to capture the steep gradient. To alleviate the meshing burden, in this work, we propose to augment the traditional finite element approximation space with a suitable ansatz to capture the steep gradient within the framework of the extended finite element method. The robustness and the accuracy of the proposed framework will be demonstrated by comparing with an overkill finite element solution. Later, the developed framework is employed to study the drifting mechanism in Lithium Lanthanum Titanium Oxide, a potential candidate for solid electrolyte material for lithium-ion batteries.

Keywords: eXtended finite element method, Nernst-Planck-Poisson equations, Solid electrolyte, Steep gradient