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Towards scalable multi-scale open-source solvers for ionic transport and electrochemistry

Tuesday, 1 June 2021 19:00 (1 hour)

In this work we present open-source solvers, based on the finite volume library OpenFOAM, for solving the Stokes-Poisson-Nernst-Planck (SPNP) system of equations for single or multi-domain ionic transfer. Many applications that involve said ionic transport, e.g reinforced concrete [1], batteries [3] and oil extraction [2], also involve heterogeneous reactions between domains. As such, interface conditions have been formulated and implemented to model this mass exchange between ionic species.

After outlining the governing equations, a dimensional analysis will be presented to note the various transport regimes capable of being seen under different scenarios by quantifying ratios between transport phenomena. We then discuss the features and capabilities of the pore-scale solvers (pnpFoam and pnpMultiFoam), as well as the heterogeneous reactive conditions (mappedChemicalKinetics). These solvers and conditions will then be verified under different test cases by comparing results against high-order spectral results obtained with the
MatLab toolbox Chebfun. Since a large number of applications of SPNP involve complex porous geometries (e.g., batteries involve a porous solid electrode flooded with fluid electrolyte), we consider the case of two- and three-dimensional randomly generated porous domain of solid and fluid [5]. Preliminary results will be presented to determine the set of geometrical parameters, through uncertainty quantification, that have significant effect on the ionic transport.

Solving at the microscale over complex porous mediums involving large scales seen in many applications is computationally intensive. Later work will be outlined to accommodate this by formulating homogenized models, parametrising the geometrical complexity, and developing therefore novel macroscopic model suitable for dominant reaction and fast ionic transfer regimes [4].

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[3] Richardson, G., Foster, J., Ranom, R., Please, C. and Ramos, A. (2020). Charge transport modelling of lithium ion batteries. arXiv:2002.00806
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Time Block Preference

Time Block B (14:00-17:00 CET)

References

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