NUMAP-FOAM Summer School 2023: Achievement

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Applied and Computational Mathematics

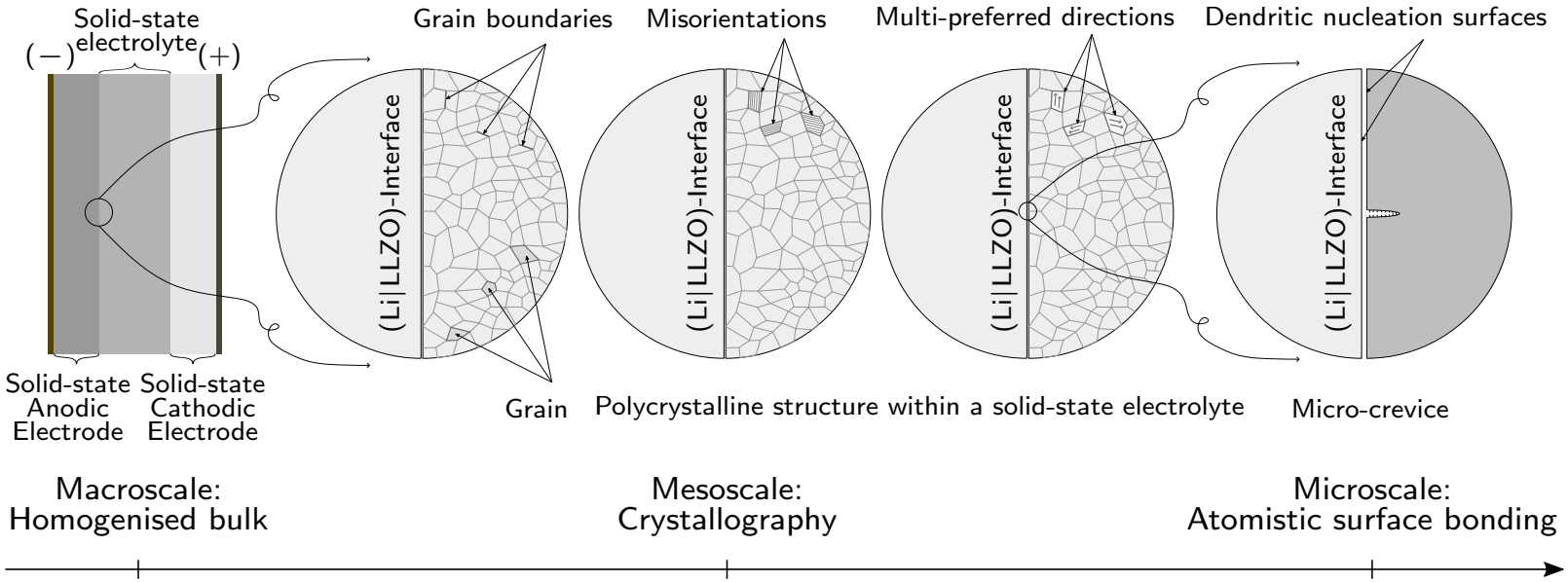
RWTH AACHEN UNIVERSITY

Cambridge, 15th September 2023

Content

1. What has been done, learned, and achieved at the NUMAP-FOAM Summer School 2023
2. Future direction and follow-up project

Main challenge: Interface analysis and numerical modelling



Find a such that the following coupled problem $\forall\, a \in \mathcal{V}$ hold:

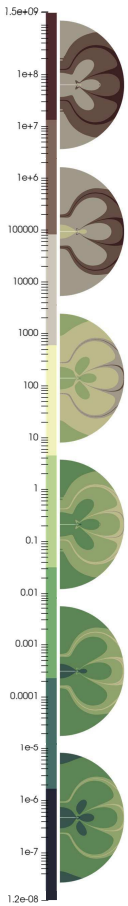
$$\rho \frac{\partial \boldsymbol{U}}{\partial t} - \nabla \cdot \left(\mathbb{C}^{T_f \phi}_{(\lambda,\mu)} : \nabla \boldsymbol{U}^{(s)} \right) + \rho \nabla V_E = \mathbf{0}, \tag{1}$$

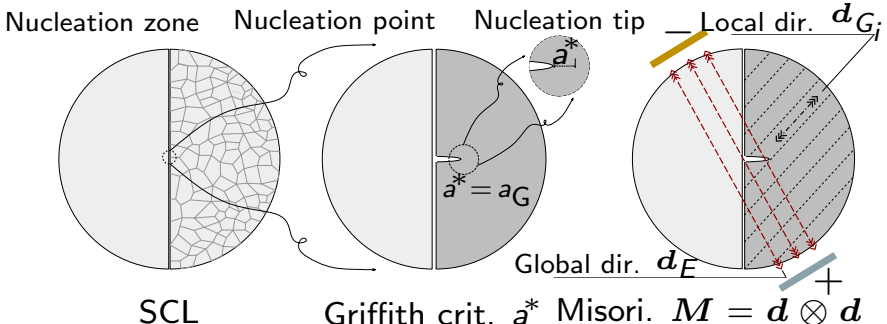
$$\text{s.t.} \quad a_{\text{Griffith}} := a^* = \arg\min_{a \in \mathcal{V}} \left\{ \iiint_{\Omega} f(a, \boldsymbol{u}, \theta, c^{m|\text{Li}^+|n}; \lambda, \mu, \boldsymbol{d}_{G_j} \otimes \boldsymbol{d}_{G_j})\, d\Omega \right.$$

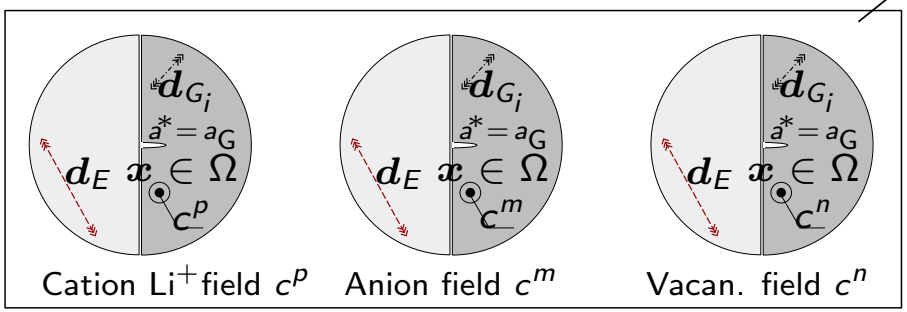
$$\left. - \iint_{\Gamma} f(a; \gamma)\, d\Gamma \right\} \tag{2}$$

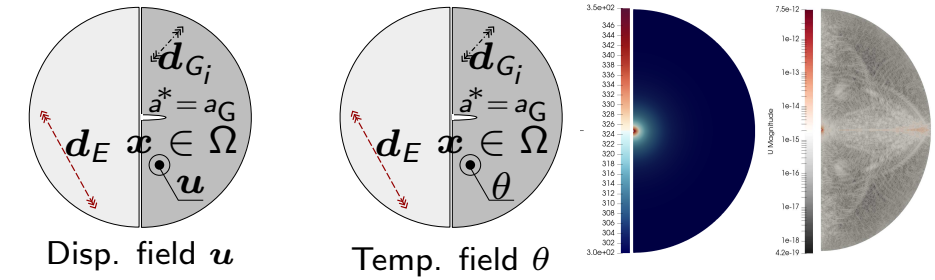
(i) Achievement

1. Compute and visualise the transport of Li-ions, Anions, Vacancies hopping at the (Li|LLZO)-Interface: ASSBFoam









Thermodynamically Consistent Model for Space-Charge-Layer Formation in a Solid Electrolyte

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$$\partial_t \rho_c = -\mathrm{div}\left(\frac{\rho}{\rho - \rho_c}\mathbf{J}_c\right)$$

$$-n^F \nabla\phi = \partial_t(\rho \mathbf{v}) + \mathrm{div}(\rho \mathbf{v} \otimes \mathbf{v}) + \nabla p$$

$$n^F = -\epsilon_0(1+\chi)\Delta\phi$$

$$\frac{\mathbf{J}_c}{m_c} = -M\left(\nabla\mu_c - \frac{m_c}{m_a}\nabla\mu_a + \left(z_c - \frac{m_c}{m_a}z_a\right)\nabla\phi - \left(1 + \frac{m_c}{m_a}\frac{n_c + n_v}{n_a}\right)\nabla\mu_v\right)$$

Set 1: (Done) Close system of $\{\boldsymbol{u}, p\}$

$$\nabla \cdot \boldsymbol{u} = 0$$

$$\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p$$

Set 2: (tbd) Close system of $\{\phi, n_c\}$

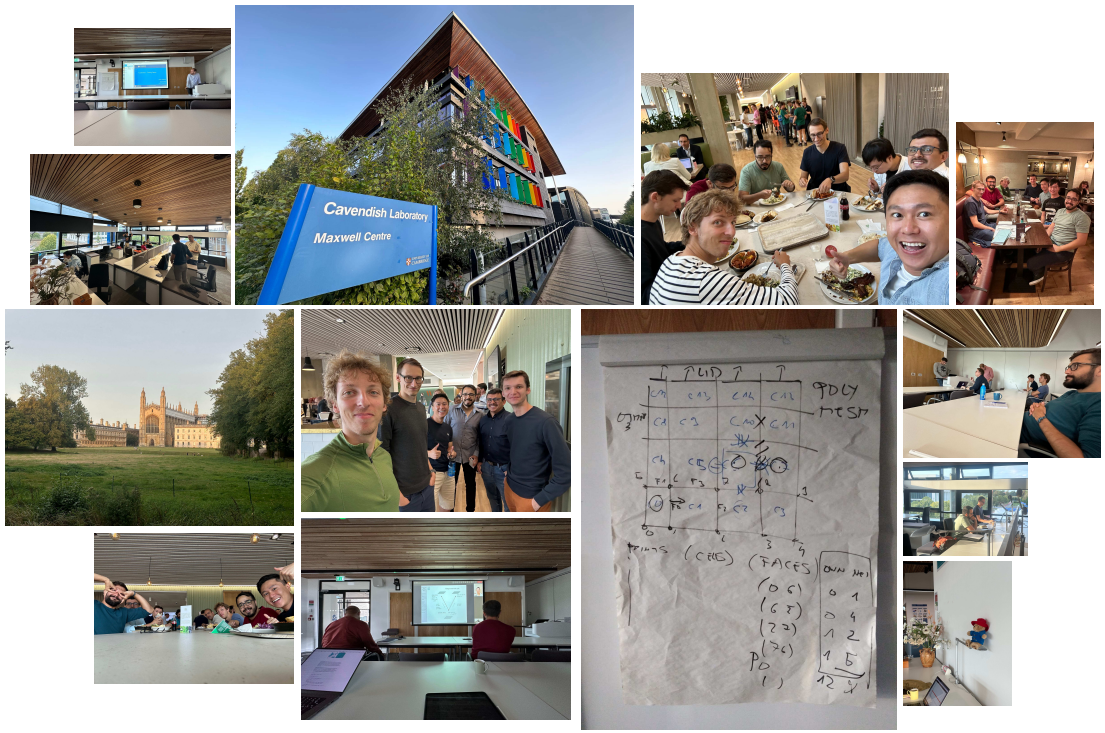
$p := \phi + \pi$

(i) EQN4 for ϕ

(ii) EQN5 for n_c

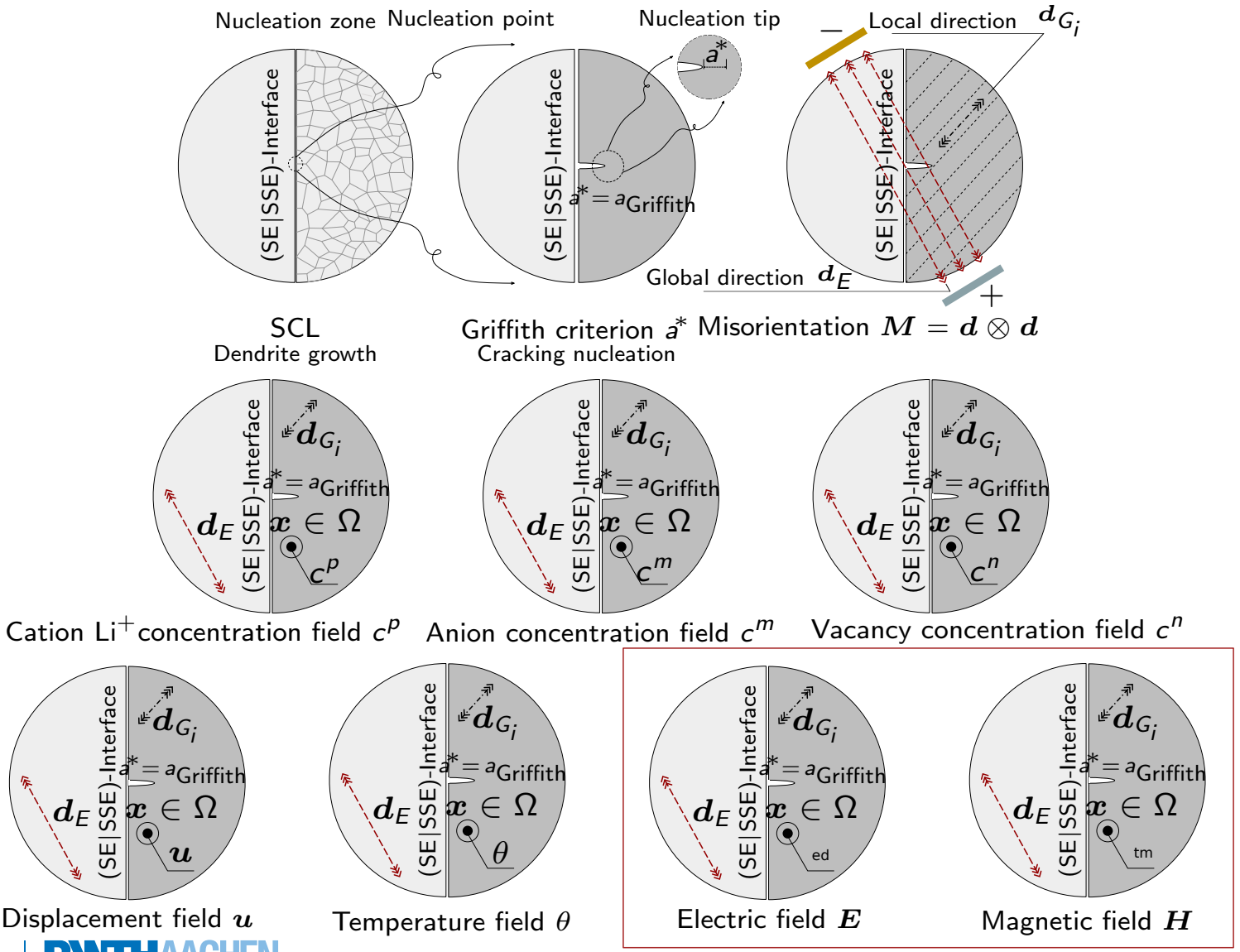
(i) Achievement

1. Learning skills, and tips & tricks about working with FOAM.
    1. FOAMPython from Robert.
    2. Possibility of FOAM with FMU/FMI from Thomas.
    3. fuelFOAM and Electrochemistry from Steffen.
    4. Insightful lectures about FOAM provided from Prof. Jasak and Tesa.
    5. Projects and works from NUMAP-FOAM 2023 Participants.
2. Extending networks and connections with FOAMers.



(ii) Future direction: Follow-up project DFG-FOR5409

1. Consistent-coupled thermodynamics to electromagnetics ASSB.



Thank you for your listening.