Mathematical modeling for all-solid-state battery: Structural tensor and the coupled electro-elastic problem

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Contents

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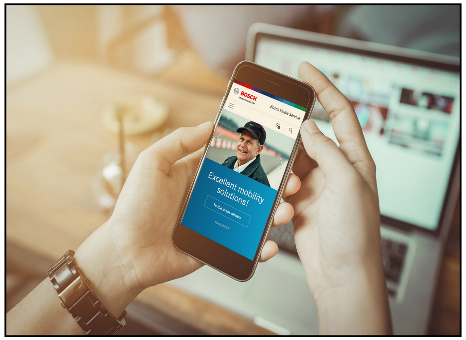
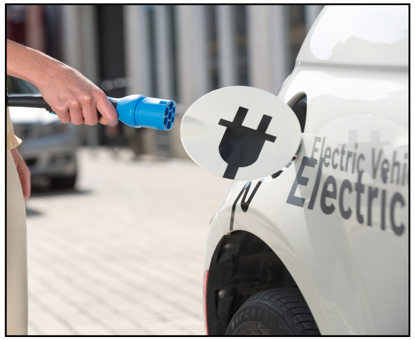
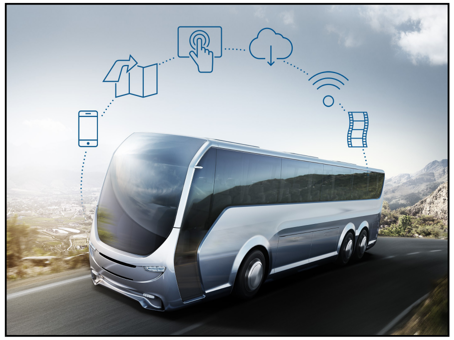
1. Motivation and Overview

Applications of Lithium-ion batteries (LIBs)







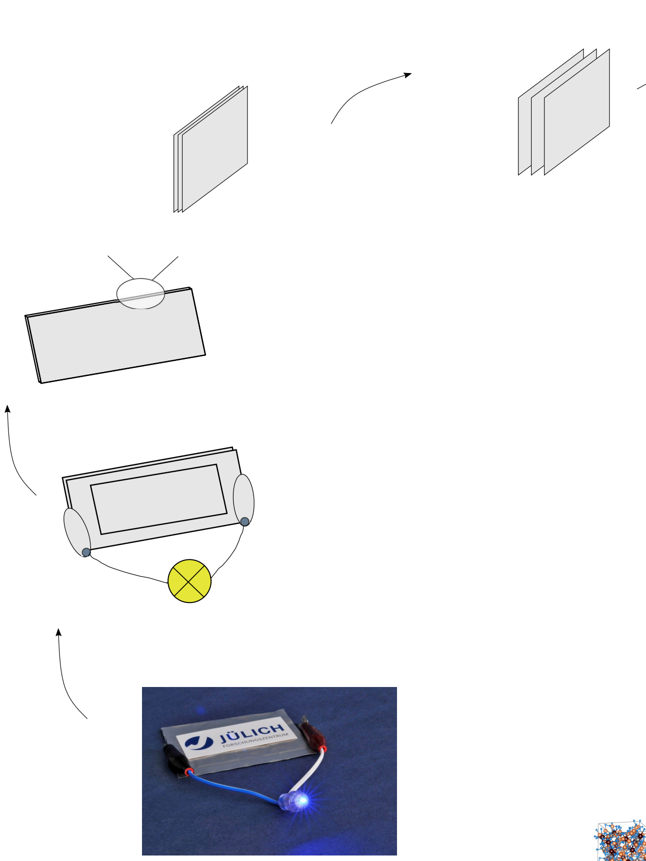
LIBs have found many applications in every energy storage system such as:

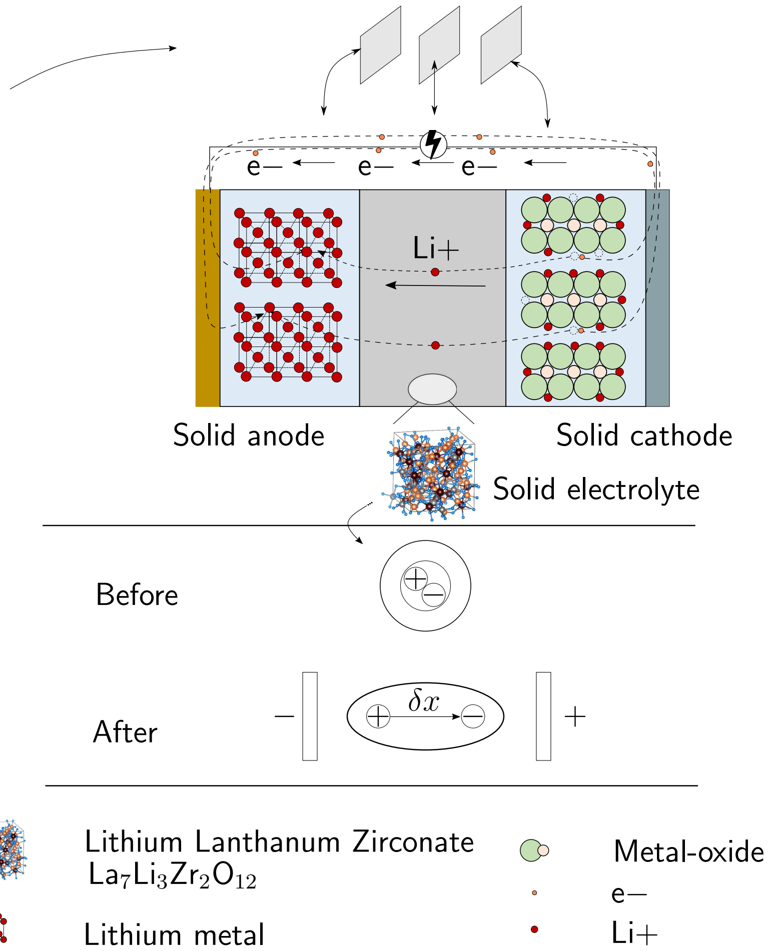
- Smartphone uses LIBs for its functionality.
- Power tools become more portable with the help of LIBs.
- Electric vehicles nowadays become more popular due to theirs zero-emission by the application of LIBs.
- Entertainment-center vehicles employ LIBs to operate their utilities properly.

Why *all-solid-state* LIBs? • high energy density • *non-flammable* • *non-leakage*

1. Motivation and Overview

Solid electrolyte is polarized under the applied electric potential.





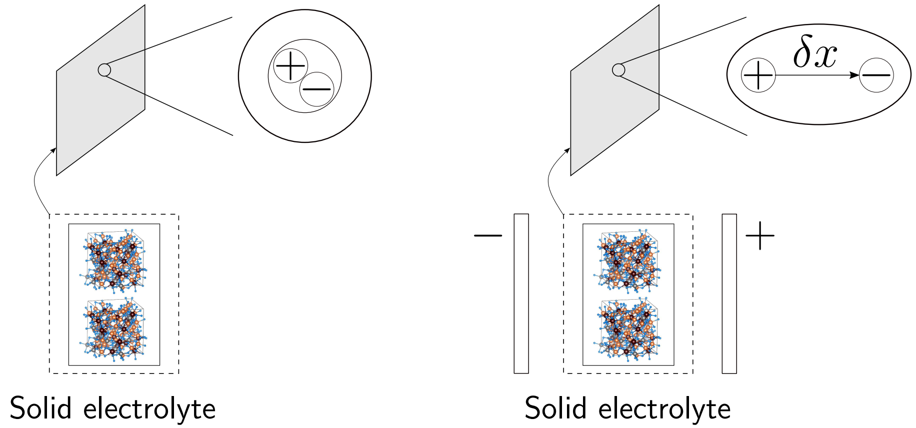
All-solid-state battery
Sample: IEK1 - Forschungszentrum Jülich

→ The polarized solid electrolyte exhibits **directional effect**.

→ The **polarized lattice** of solid electrolyte causes **overall deformation** in structure.

1. Motivation and Overview

Polarization illustration



Background and overview:

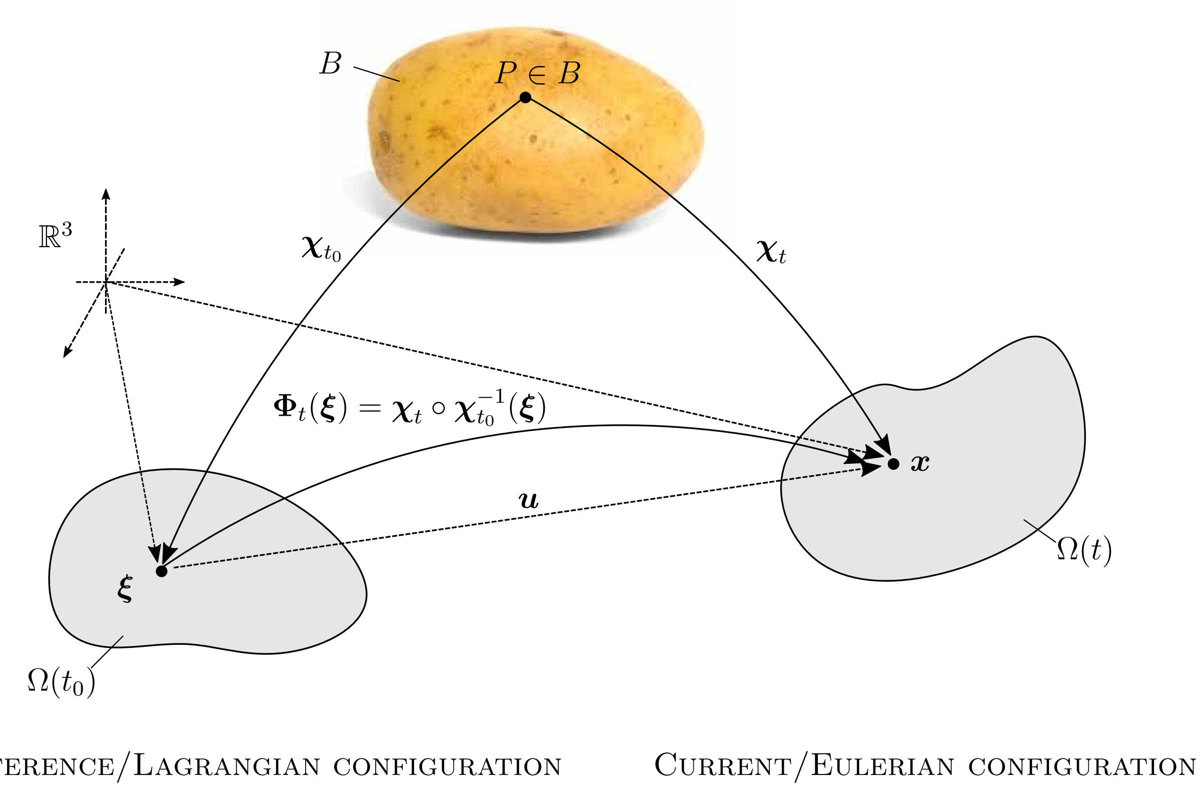
- Thermodynamically consistent model for space-charge-layer formation in a solid electrolyte; S. Braun et. al. [2015].
- Mathematical modeling in Continuum Physics; Lecture note; M. Torrilhon [2018].
- Introduction to Electrodynamics; D. Griffiths; Electromagnetic theory; A. Kovetz.

Goals:

- A thermodynamic consistent formulation for constitutive relations.
- Capture the directional effect and electro-elastic phenomena.
- Numerical implementation based on open source.

2. Mathematical modeling of coordinate-free structure-tensor-based material

Continuum physics kinematics



Def: The tensor $\boldsymbol{F} := \frac{\partial \boldsymbol{\Phi}(\boldsymbol{\xi},t)}{\partial \boldsymbol{\xi}}$ or $F_{ij} = \frac{\partial \Phi_i(\boldsymbol{\xi},t)}{\partial \xi_j}$ is called the *deformation gradient*.

Displacement vector: $\boldsymbol{u} = \boldsymbol{x} - \boldsymbol{\xi}$

Deformation gradient using displacement vector: $\boldsymbol{F} = \boldsymbol{I} + \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}}$

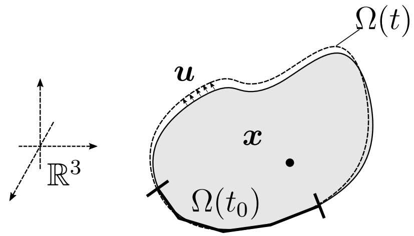
Right and left Cauchy-Green deformation tensors: $\boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F}$; $\boldsymbol{B} = \boldsymbol{F}\boldsymbol{F}^T$

Green-Lagrange strain tensor: $\boldsymbol{E} = 1/2(\boldsymbol{C} - \boldsymbol{I}) = 1/2(\boldsymbol{F}^T\boldsymbol{F} - \boldsymbol{I})$

2. Mathematical modeling of coordinate-free structure-tensor-based material

Continuum physics kinematics

Consider Green-Lagrange strain tensor $\boldsymbol{E}$ where the displacement is small $\leftrightarrow$ $\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}} = \mathcal{O}(\varepsilon),\ \varepsilon \ll 1$:



Displacement $\boldsymbol{u}$

$$\boldsymbol{E} = \frac{1}{2}(\boldsymbol{F}^T\boldsymbol{F} - \boldsymbol{I}) = \frac{1}{2}\left[\left(\boldsymbol{I} + \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}}\right)^T \left(\boldsymbol{I} + \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}}\right) - \boldsymbol{I}\right] = \frac{1}{2}\left[\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}} + \left(\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}}\right)^T + \underbrace{\left(\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}}\right)^T \left(\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}}\right)}_{\text{Neglected}}\right]$$

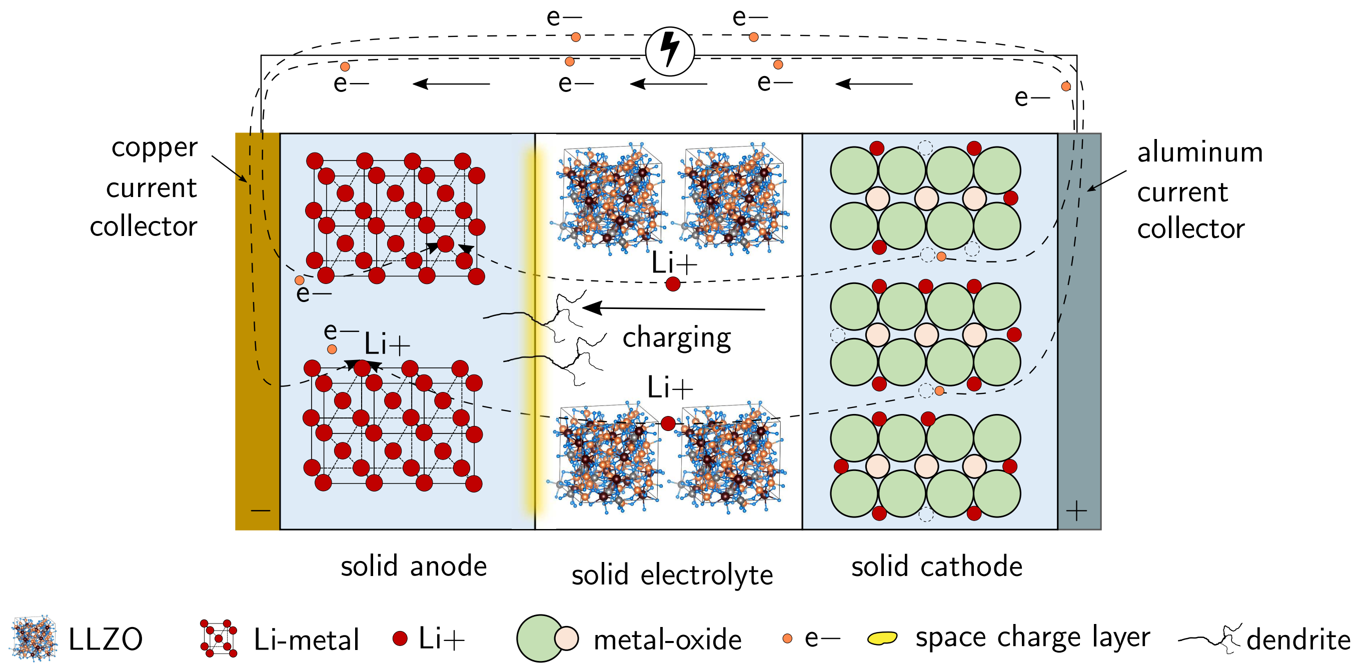
leading to infinitesimal strain tensor

$$\boxed{\boldsymbol{\varepsilon} := \frac{1}{2}\left[\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}} + \left(\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}}\right)^T\right]}$$

$\rightarrow$ This kinematic relation is used for the model of solid electrolyte.

2. Mathematical modeling of coordinate-free structure-tensor-based material

Continuum physics kinematics



$$\boldsymbol{E} = \frac{1}{2}(\boldsymbol{F}^T\boldsymbol{F} - \boldsymbol{I}) = \frac{1}{2}\left[\left(\boldsymbol{I} + \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}}\right)^T \left(\boldsymbol{I} + \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}}\right) - \boldsymbol{I}\right] = \frac{1}{2}\left[\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}} + \left(\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}}\right)^T + \underbrace{\left(\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}}\right)^T \left(\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}}\right)}_{\text{Keep}}\right]$$

→ The solid electrolyte is mixed with polymer in order to buffer/prevent dendrite formation (IEK2-FZ Jülich).
→ The solid electrolyte with reinforced polymer exhibits finite strain behavior.

2. Mathematical modeling of coordinate-free structure-tensor-based material

Continuum physics kinematics

- Small strain

$$\boxed{\boldsymbol{\varepsilon} := \frac{1}{2}\left[\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}} + \left(\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}}\right)^T\right]}$$

$\rightarrow$ Kinematic relation for small strain has implied that $\boldsymbol{F}$ deviates only from the identity $\boldsymbol{I}$, which means $\boldsymbol{F} \approx \boldsymbol{I}$.

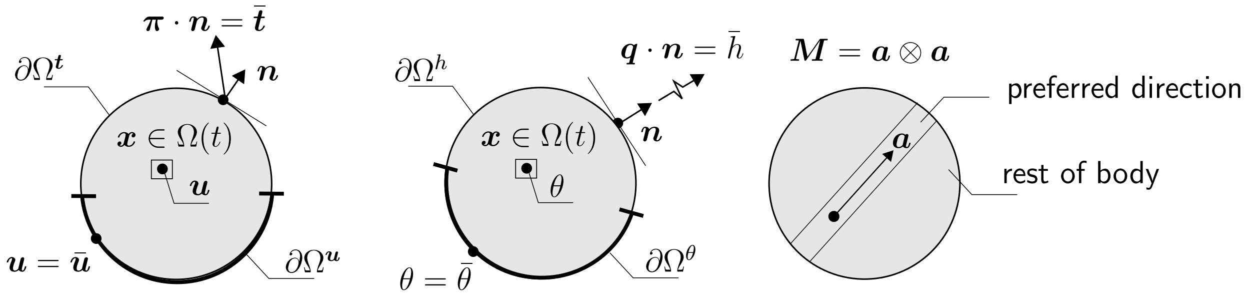
- Cauchy's stress theorem $\boldsymbol{t}(\boldsymbol{x}, t; \boldsymbol{n}) := \boldsymbol{T}(\boldsymbol{x}, t) \cdot \boldsymbol{n}$ and the corresponding stress tensors

Cauchy stress	$\boldsymbol{T}$
Kirchhoff stress	$\boldsymbol{\tau} := J\boldsymbol{T}$
First Piola-Kirchhoff stress	$\boldsymbol{P} := J\boldsymbol{T}\boldsymbol{F}^{-T} = \boldsymbol{\tau}\boldsymbol{F}^{-T}$
Second Piola-Kirchhoff stress	$\boldsymbol{S} := \boldsymbol{F}^{-1}\boldsymbol{P} = \boldsymbol{F}^{-1}\boldsymbol{\tau}\boldsymbol{F}^{-T}$

$\rightarrow$ There is one kind of mechanical stress left:

$$\boxed{\boldsymbol{\pi} := \boldsymbol{P} \approx \boldsymbol{S} \approx \boldsymbol{\tau} \approx \boldsymbol{T}}$$

Primary fields



DISPLACEMENT FIELD $\boldsymbol{u}$ TEMPERATURE FIELD θ STRUCTURE TENSOR $\boldsymbol{M}$

• Primary field variables and their gradients

Displacement field and temperature field

$$\boldsymbol{u} : \begin{cases} \Omega(t) \times \mathbb{R}_+ \to \mathbb{R}^3, \\ (\boldsymbol{x}, t) \mapsto \boldsymbol{u}(\boldsymbol{x}, t), \end{cases} \quad \text{and} \quad \theta : \begin{cases} \Omega(t) \times \mathbb{R}_+ \to \mathbb{R}, \\ (\boldsymbol{x}, t) \mapsto \theta(\boldsymbol{x}, t), \end{cases}$$

Gradient of displacement field $\boldsymbol{u}$ and temperature field θ

$$\boldsymbol{\varepsilon} = \nabla_s \boldsymbol{u}(\boldsymbol{x}, t), \qquad \boldsymbol{g} := \nabla\theta(\boldsymbol{x}, t).$$

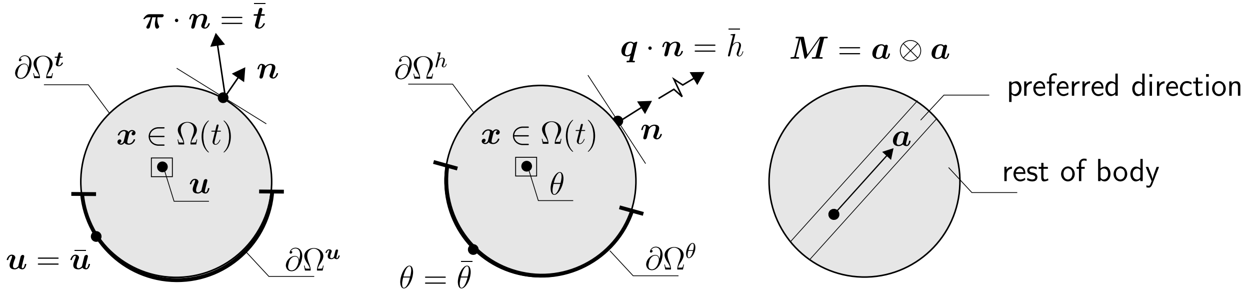
Structure tensor $\boldsymbol{M} = \boldsymbol{a} \otimes \boldsymbol{a}$

$$\mathbb{G} := \left\{ \boldsymbol{Q}_{||_{\boldsymbol{a}}}, \boldsymbol{Q}_{\perp_{\boldsymbol{a}}} \right\} \subset \mathcal{O}(3)$$

$$\boxed{\hat{\Psi}(\boldsymbol{\varepsilon}, \boldsymbol{M}) = \hat{\Psi}(\boldsymbol{Q}\boldsymbol{\varepsilon}\boldsymbol{Q}^T, \boldsymbol{Q}\boldsymbol{M}\boldsymbol{Q}^T) = \hat{\Psi}(\boldsymbol{\varepsilon}, \boldsymbol{M}) \quad \forall\, \boldsymbol{Q} \in \mathbb{G}}$$

2. Mathematical modeling of coordinate-free structure-tensor-based material

Local balance law of the coupled problem in current configuration



DISPLACEMENT FIELD $\boldsymbol{u}$ TEMPERATURE FIELD θ STRUCTURE TENSOR $\boldsymbol{M}$

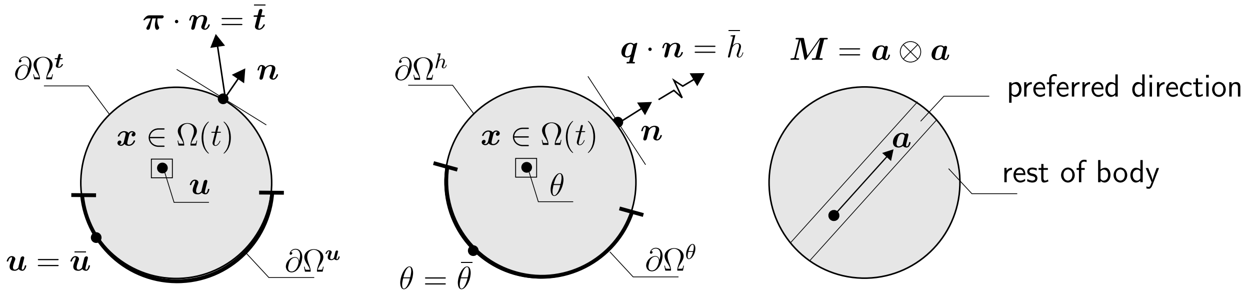
• Summary of local balance laws

Local balance laws governing the infinitesimal elasticity embedded structural tensor

Balance of mass	$\dot{\rho} + \rho \operatorname{div} \boldsymbol{v} = 0$
Balance of linear momentum	$\rho \dot{v} = \operatorname{div} \boldsymbol{\pi} + \rho \boldsymbol{b}$
Balance of angular momentum	$\boldsymbol{\pi}^T = \boldsymbol{\pi}$
Balance of energy	$\rho \dot{e} = \boldsymbol{\pi} : \dot{\boldsymbol{\varepsilon}} + \rho r - \operatorname{div} \boldsymbol{q}$

2. Mathematical modeling of coordinate-free structure-tensor-based material

Local balance law of the coupled problem in reference configuration



DISPLACEMENT FIELD $\boldsymbol{u}$ TEMPERATURE FIELD θ STRUCTURE TENSOR $\boldsymbol{M}$

- **Entropy inequality**

$$\boxed{\text{Entropy inequality} \quad \rho\mathcal{D} := \underbrace{\boldsymbol{\pi} : \dot{\boldsymbol{\varepsilon}} - \rho\eta\dot{\theta} - \rho\dot{\Psi}}_{\rho\mathcal{D}_{\text{loc}}} \underbrace{-\frac{1}{\theta}\boldsymbol{q} \cdot \nabla\theta}_{\rho\mathcal{D}_{\text{diff}}} \geq 0}$$

- **Sharper restriction postulation**

Local action term $\rho\mathcal{D}_{\text{loc}}$ and diffusion term $\rho\mathcal{D}_{\text{diff}}$ are enforced as follows

$$\boxed{\begin{aligned} &\rho\mathcal{D}_{\text{loc}} := \boldsymbol{\pi} : \dot{\boldsymbol{\varepsilon}} - \rho\eta\dot{\theta} - \rho\dot{\Psi} \geq 0 \\ &\rho\mathcal{D}_{\text{diff}} := -\frac{1}{\theta}\boldsymbol{q} \cdot \nabla\theta \geq 0 \end{aligned}}$$

$\rightarrow$ Thermodynamic consistency is satisfied via this sharper restriction postulation.

2. Mathematical modeling of coordinate-free structure-tensor-based material

- **Free energy function**

$$\boxed{\Psi(\boldsymbol{\varepsilon}, \boldsymbol{M}) = \tilde{\Psi}(I_1, I_2, I_4, I_5) = \frac{1}{2}\lambda I_1^2 + \mu_T I_2 + \alpha I_1 I_4 + 2(\mu_L - \mu_T) I_5 + \frac{1}{2}\beta I_4^2}$$

where $I_1 = \mathrm{tr}[\varepsilon], \quad I_2 = \mathrm{tr}[\varepsilon^2], \quad I_3 = \mathrm{tr}[\varepsilon^3], \quad I_4 = \mathrm{tr}[\varepsilon \boldsymbol{M}], \quad I_5 = \mathrm{tr}[\varepsilon^2 \boldsymbol{M}]$

- **Constitutive equations**

Stress tensor

$$\begin{aligned}\boldsymbol{\pi} = \partial_{\boldsymbol{\varepsilon}} \tilde{\Psi} &= (\lambda I_1 + \alpha I_4)\mathbf{1} + 2\mu_T \boldsymbol{\varepsilon} + (\lambda I_1 + \alpha I_4)\boldsymbol{M} + 2(\mu_L - \mu_T)(\boldsymbol{M}\boldsymbol{\varepsilon} + \boldsymbol{\varepsilon}\boldsymbol{M}) \\ &= \underbrace{\lambda I_1 \mathbf{1} + 2\mu_T \boldsymbol{\varepsilon}}_{\text{isotropic part}} + \underbrace{\alpha(I_4 \mathbf{1} + I_1 \boldsymbol{M}) + 2(\mu_L - \mu_T)(\boldsymbol{M}\boldsymbol{\varepsilon} + \boldsymbol{\varepsilon}\boldsymbol{M}) + \beta I_4 \boldsymbol{M}}_{\text{anisotropic part}}\end{aligned}$$

Tangent modulus

$$\mathbb{C} = \partial_{\varepsilon\varepsilon} \tilde{\Psi} = \partial_{\varepsilon} \boldsymbol{\pi} = \lambda \mathbf{1} \otimes \mathbf{1} + 2\mu_T \mathbb{I} + \alpha(\mathbf{1} \otimes \boldsymbol{M} + \boldsymbol{M} \otimes \mathbf{1}) + 2(\mu_L - \mu_T)\mathbb{I}_{\boldsymbol{a}} + \beta \boldsymbol{M} \otimes \boldsymbol{M}$$

where

$$\begin{aligned}\mathbb{I}_{\boldsymbol{a}} = [\mathbb{I}_{\boldsymbol{a}}]_{ijkl} &= \frac{1}{2}(M_{ik}\delta_{jl} + M_{il}\delta_{jk} + M_{jl}\delta_{ik} + M_{jk}\delta_{il}) \\ &= \frac{1}{2}(a_i \delta_{jl} a_k + a_i \delta_{jk} a_l + a_j \delta_{ik} a_l + a_j \delta_{il} a_k)\end{aligned}$$

3. Numerical implementation and representative examples from first approach

Problem to solve

PDE	$\pi_{ij,j} + \rho b_i = 0$
Constitutive relation	$\pi_{ij} = \mathbb{C}_{ijkl}\ \varepsilon_{kl}$
Kinematic relation	$\varepsilon_{kl} = \dfrac{1}{2}\left(\dfrac{\partial u_k}{\partial x_l} + \dfrac{\partial u_l}{\partial x_k}\right)$
Dirichlet BC	$u_i = \bar{u}_i$ on $\partial\Omega_{u_i}$
Neumann BC	$\pi_{ij}n_j = t_i$ on $\partial\Omega_{t_i}$

where
$$\mathbb{C}_{ijkl} = \lambda\delta_{ij}\delta_{kl} + 2\mu_T\mathbb{I}_{ijkl} + \alpha(\delta_{ij}M_{kl} + M_{ij}\delta_{kl}) + 2(\mu_L - \mu_T)\,[\mathbb{I}_{\boldsymbol{a}}]_{ijkl} + \beta M_{ij}M_{kl}$$
$$[\mathbb{I}_{\boldsymbol{a}}]_{ijkl} = \frac{1}{2}(a_i\delta_{jl}a_k + a_i\delta_{jk}a_l + a_j\delta_{ik}a_l + a_j\delta_{il}a_k)$$
$$\mathbb{I}_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$$

Functions defined

```
{#include <deal.II>
using namespace dealii;
 public: FEM (); ~FEM();
    //Setup
    void general_setup();
    void meshing();
    void assembling();
    //Boundary conditions and Initial conditions
    void boundary_conditions();
    void initial_conditions();
    //Solving
    void solving_steady();
    void solving_transient();
    //Output
    void output_steady();
    void output_transient();
    //Other useful functions
    double C(unsigned int i,unsigned int j,unsigned int k,unsigned int l);
}
```

3. Numerical implementation and representative examples from first approach

Local stiffness matrix K

```
{Klocal = 0.0;
for (unsigned int q=0; q<num_quad_pts; ++q){
    for (unsigned int M=0; M<nodes_per_elem; M++){
        for (unsigned int i=0; i<dim; i++){
            for (unsigned int N=0; B<nodes_per_elem; N++){
                for (unsigned int k=0; k<dim; k++){
                    for (unsigned int j=0; j<dim; j++){
                        for (unsigned int l=0; l<dim; l++){
                        Klocal[3*M+i][3*N+k] += fe_values.shape_grad(3*M+i,q)[j]
                      *C(i,j,k,l)*fe_values.shape_grad(3*N+k,q)[l]*fe_values.JxW(q);
                       }}}}}}}
}
```

3. Numerical implementation and representative examples from first approach

Local mass matrix M

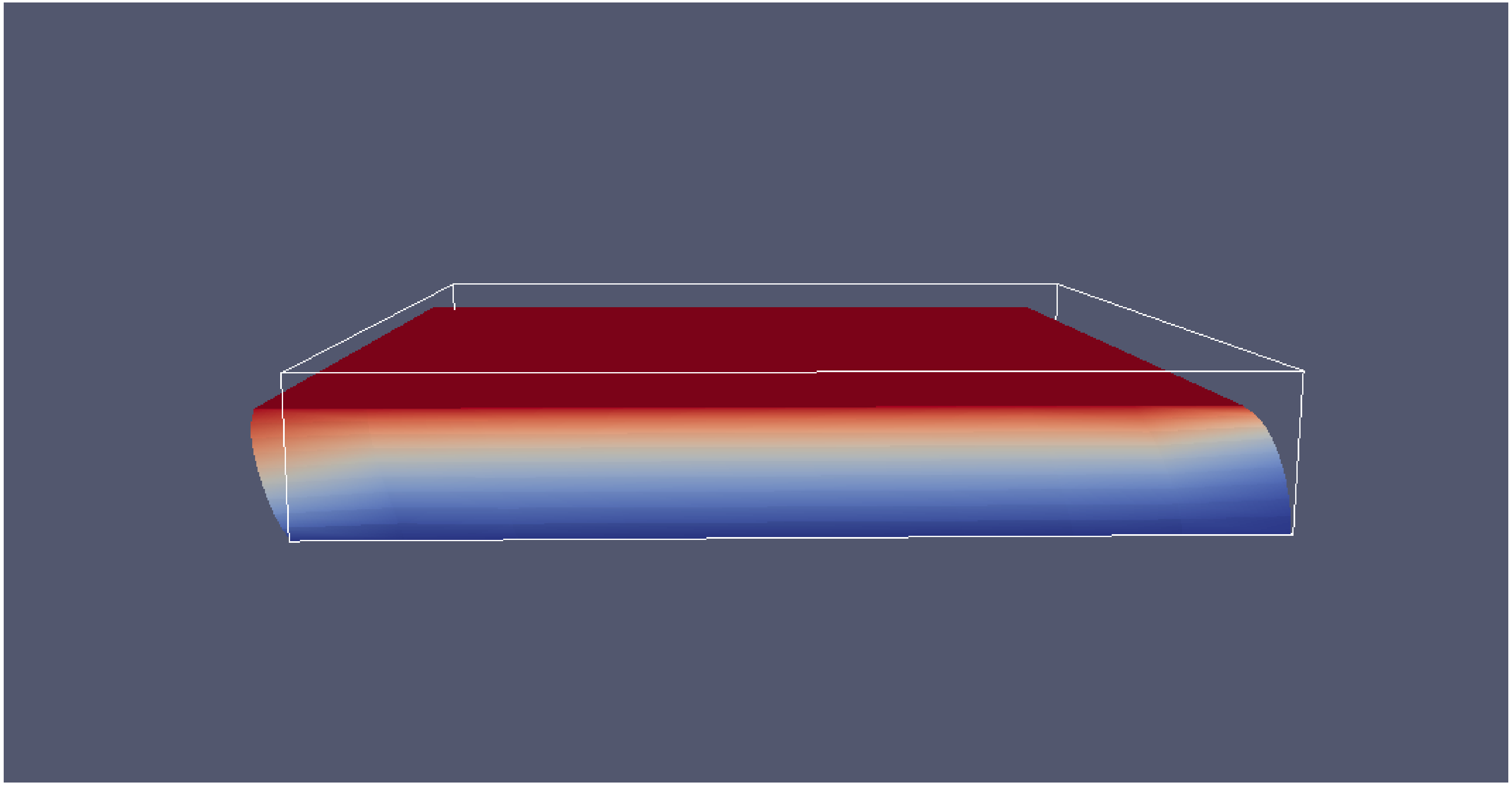
```
{Mlocal = 0.0;
for(unsigned int q=0; q<num_quad_pts; q++){
    for(unsigned int M=0; M<nodes_per_elem; M++){
        for(unsigned int i=0; i<dim; i++){
            for(unsigned int N=0; N<nodes_per_elem; N++){
                Mlocal[3*M+i][3*N+i] += fe_values.shape_value(3*M+i,q)
                        *fe_values.shape_value(3*N+i,q)*fe_values.JxW(q)*rho;
          }}}}
}
```

Local force vector F

```
{Flocal = 0.0;
[...]
            Flocal[3*M+i] += fe_face_values.shape_value(3*M+i,q)
                    *fe_face_values.JxW(q)*tbar[i];
}
```

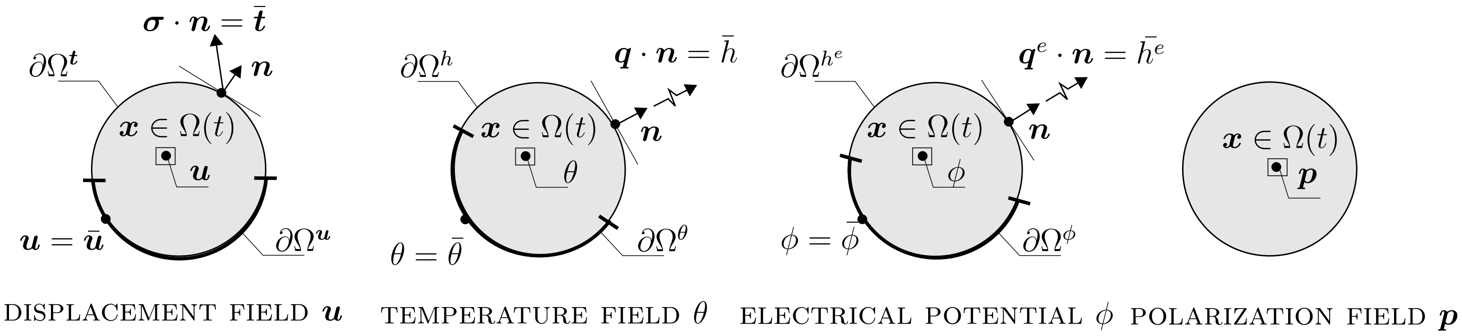
3. Numerical implementation and representative examples from first approach

Result: 3D



- The solid electrolyte exhibits anisotropic property due to coordinate free structure tensor $\boldsymbol{M}$.
- Numerical analysis is aimed for the next step.

Primary fields of electro-elastic coupled problem



• Primary field variables and their gradients

Displacement field, temperature field, electrical potential and polarization field

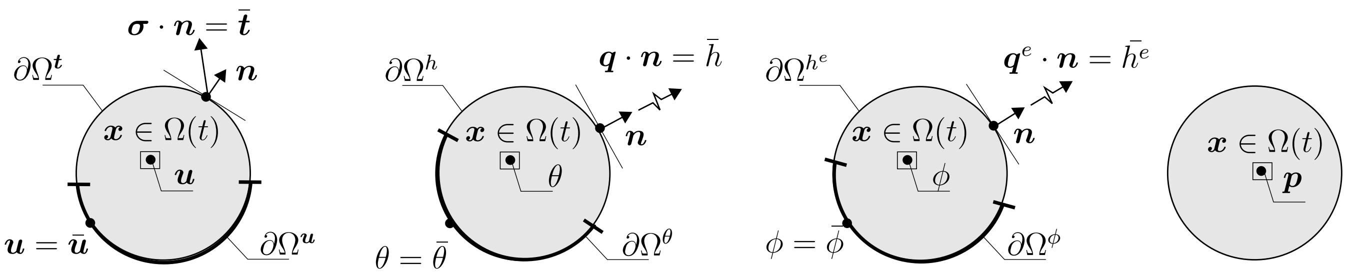
$$\boldsymbol{u} : \begin{cases} \Omega \times \mathbb{R}_+ \to \mathbb{R}^3, \\ (\boldsymbol{x}, t) \mapsto \boldsymbol{u}(\boldsymbol{x}, t), \end{cases} \qquad \theta : \begin{cases} \Omega \times \mathbb{R}_+ \to \mathbb{R}, \\ (\boldsymbol{x}, t) \mapsto \theta(\boldsymbol{x}, t), \end{cases} \qquad \phi : \begin{cases} \Omega \times \mathbb{R}_+ \to \mathbb{R}, \\ (\boldsymbol{x}, t) \mapsto \phi(\boldsymbol{x}, t), \end{cases} \qquad \boldsymbol{p} : \begin{cases} \Omega \times \mathbb{R}_+ \to \mathbb{R}, \\ (\boldsymbol{x}, t) \mapsto \boldsymbol{p}(\boldsymbol{x}, t). \end{cases}$$

Gradient of deformation field $\boldsymbol{u}$, temperature field θ, electrical potential ϕ and polarization $\boldsymbol{p}$

$$\boldsymbol{\varepsilon} = \nabla_s \boldsymbol{u}(\boldsymbol{x}, t), \qquad \boldsymbol{g} := \nabla\theta(\boldsymbol{x}, t), \qquad \mathbb{e} := -\nabla\phi(\boldsymbol{x}, t), \qquad \mathbb{p} := \nabla\boldsymbol{p}(\boldsymbol{x}, t).$$

4. Mathematical model of electro-elastic coupled problem - Second approach

Balance laws of the coupled problem



DISPLACEMENT FIELD $\boldsymbol{u}$ TEMPERATURE FIELD θ ELECTRICAL POTENTIAL ϕ POLARIZATION FIELD $\boldsymbol{p}$

• Conservation of mass - No modified

Global and local form:

$$\frac{d}{dt}\int_{\Omega(t)} \rho \, dv = 0; \qquad \therefore \boxed{\dot{\rho} + \rho \operatorname{div} \boldsymbol{v} = 0}$$

• Conservation of linear momentum - Modified

Global:

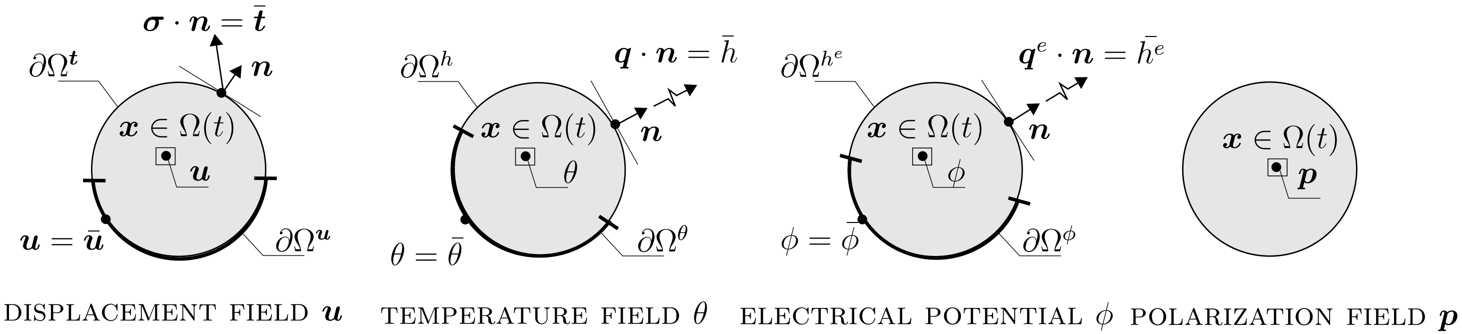
$$\frac{d}{dt}\int_{\Omega(t)} \rho \boldsymbol{v} dv = \int_{\Omega(t)} \rho \boldsymbol{b} \, dv + \oint_{\partial\Omega(t)} \boldsymbol{t} \, da \boxed{+ \int_{\Omega(t)} \rho \boldsymbol{b}^e dv} = \int_{\Omega(t)} \rho \boldsymbol{b} \, dv + \oint_{\partial\Omega(t)} \boldsymbol{\sigma}_C \cdot \boldsymbol{n} \, da + \int_{\Omega(t)} \rho \boldsymbol{b}^e dv$$

Local:

$$\therefore \boxed{\rho \dot{\boldsymbol{v}} = \operatorname{div} \boldsymbol{\sigma}_C + \rho \boldsymbol{b} + \rho \boldsymbol{b}^e}$$

4. Mathematical model of electro-elastic coupled problem - Second approach

Balance laws of the coupled problem



• Conservation of angular momentum - Modified

Global:

$$\frac{d}{dt}\int_{\Omega(t)}\boldsymbol{x}\times\rho\boldsymbol{v}\;dv=\underbrace{\int_{\Omega(t)}\boldsymbol{x}\times\rho\boldsymbol{b}\;dv}_{\text{RHS1}}+\underbrace{\oint_{\partial\Omega(t)}\boldsymbol{x}\times(\boldsymbol{\sigma}_C\cdot\boldsymbol{n})\;da}_{\text{RHS2}}\;\boxed{+\underbrace{\int_{\Omega(t)}\rho\boldsymbol{c}\;dv}_{\text{Coupling term}}}$$

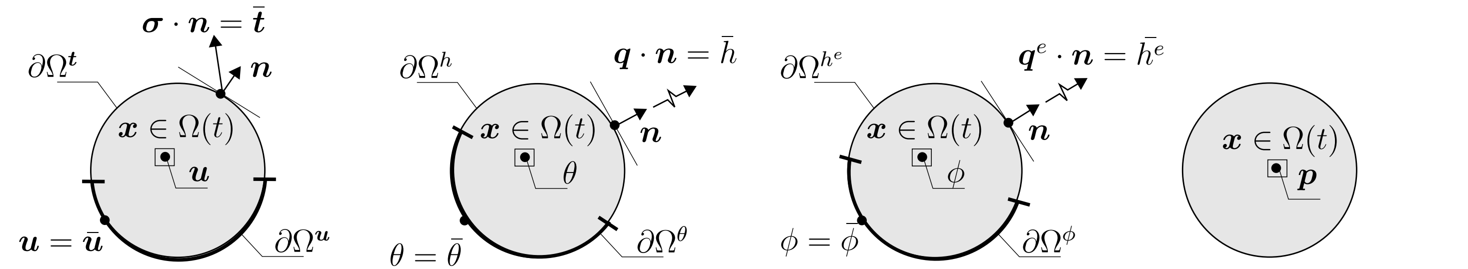
$$\text{LHS}\;\rightarrow\;\boldsymbol{\kappa}\times\frac{d}{dt}\int_{\Omega(t)}\boldsymbol{x}\times\rho\boldsymbol{v}\;dv=\left(\int_{\Omega(t)}(\boldsymbol{x}\otimes\rho\dot{\boldsymbol{v}}-\rho\dot{\boldsymbol{v}}\otimes\boldsymbol{x})dv\right)\boldsymbol{\kappa}$$

$$\text{RHS1}\;\rightarrow\;\boldsymbol{\kappa}\times\int_{\Omega(t)}\boldsymbol{x}\times\rho\boldsymbol{b}\;dv=\left(\int_{\Omega(t)}(\boldsymbol{x}\otimes\rho\boldsymbol{b}-\rho\boldsymbol{b}\otimes\boldsymbol{x})\;dv\right)\boldsymbol{\kappa}$$

$$\text{RHS2}\;\rightarrow\;\boldsymbol{\kappa}\times\oint_{\partial\Omega(t)}\boldsymbol{x}\times(\boldsymbol{\sigma}_C\cdot\boldsymbol{n})\;da=\left(\int_{\Omega(t)}(\boldsymbol{x}\otimes\operatorname{div}\boldsymbol{\sigma}_C-\operatorname{div}\boldsymbol{\sigma}_C\otimes\boldsymbol{x}-(\operatorname{grad}\boldsymbol{x})\boldsymbol{\sigma}_C^T+(\operatorname{grad}\boldsymbol{x})\boldsymbol{\sigma}_C)\;dv\right)\boldsymbol{\kappa}$$

4. Mathematical model of electro-elastic coupled problem - Second approach

Balance laws of the coupled problem



• Conservation of angular momentum - Modified

Global:

$$\frac{d}{dt}\int_{\Omega(t)}\boldsymbol{x}\times\rho\boldsymbol{v}\;dv=\underbrace{\int_{\Omega(t)}\boldsymbol{x}\times\rho\boldsymbol{b}\;dv}_{\text{RHS1}}+\underbrace{\oint_{\partial\Omega(t)}\boldsymbol{x}\times(\boldsymbol{\sigma}_C\cdot\boldsymbol{n})\;da}_{\text{RHS2}}\;\boxed{\underbrace{+\int_{\Omega(t)}\rho\boldsymbol{c}\;dv}_{\text{Coupling term}}}$$

(LHS $-$ RHS1 $-$ RHS2)$\boldsymbol{\kappa}=\boldsymbol{\kappa}\times$ Coupling term

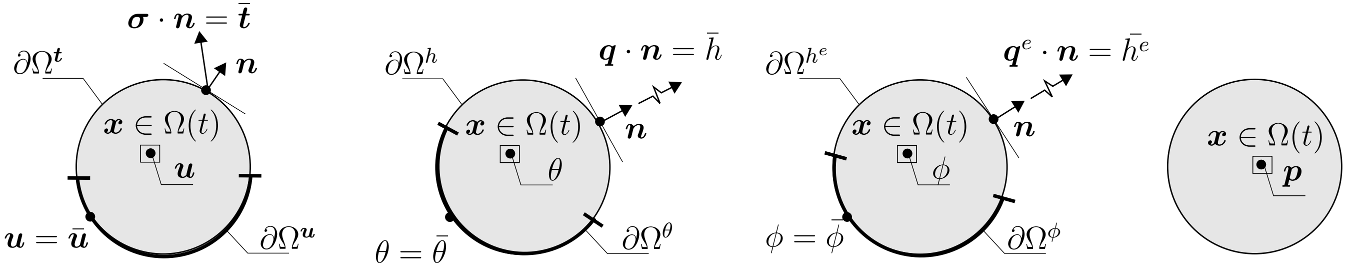
$$\left\{\int_{\Omega(t)}\left\{\boldsymbol{x}\otimes(\rho(\dot{v}-\boldsymbol{b}-\boldsymbol{b}^e)-\operatorname{div}\boldsymbol{\sigma}_C)-(\rho(\dot{v}-\boldsymbol{b}-\boldsymbol{b}^e)-\operatorname{div}\boldsymbol{\sigma}_C)\otimes\boldsymbol{x}-\boldsymbol{\sigma}_C^T+\boldsymbol{\sigma}_C\right\}dv\right\}\boldsymbol{\kappa}=\boldsymbol{\kappa}\times\int_{\Omega(t)}\rho\boldsymbol{c}\;dv$$

Local:

$$\therefore\;\boxed{\overset{axial}{\boldsymbol{t}}\;\text{skew}[\boldsymbol{\sigma}_C]=\rho\boldsymbol{c}}\;\rightarrow\text{ Loss of symmetric property in Cauchy stress }\boldsymbol{\sigma}.$$

4. Mathematical model of electro-elastic coupled problem - Second approach

Balance laws of the coupled problem



DISPLACEMENT FIELD $\boldsymbol{u}$ TEMPERATURE FIELD θ ELECTRICAL POTENTIAL ϕ POLARIZATION FIELD $\boldsymbol{p}$

- **Energy balance - Modified**

Global:

$$\frac{d}{dt}\int_{\Omega(t)}\left[\frac{1}{2}\rho\left|\boldsymbol{v}\right|^2 + \rho e\right]\, dv = \int_{\Omega(t)}\rho\boldsymbol{b}\cdot\boldsymbol{v}\, dv + \oint_{\partial\Omega(t)}\boldsymbol{t}\cdot\boldsymbol{v}\, da$$

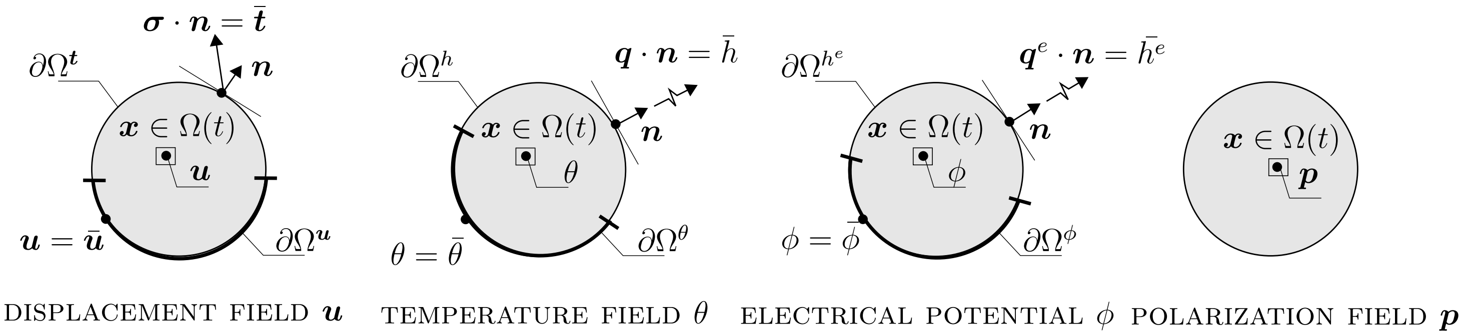
$$+\int_{\Omega(t)}\rho r\, dv - \oint_{\partial\Omega(t)}\boldsymbol{q}\cdot\boldsymbol{n}\, da \boxed{+\int_{\Omega(t)}\rho r^e\, dv}$$

Local:

$$\therefore \boxed{\rho\dot{e} = \boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}} + \rho r + \rho r^e - \operatorname{div}\boldsymbol{q}}$$

4. Mathematical model of electro-elastic coupled problem - Second approach

Balance laws of the coupled problem



• Summary of local balance laws

Local balance laws governing the coupled electro-elastic problem in $\Omega(t)$

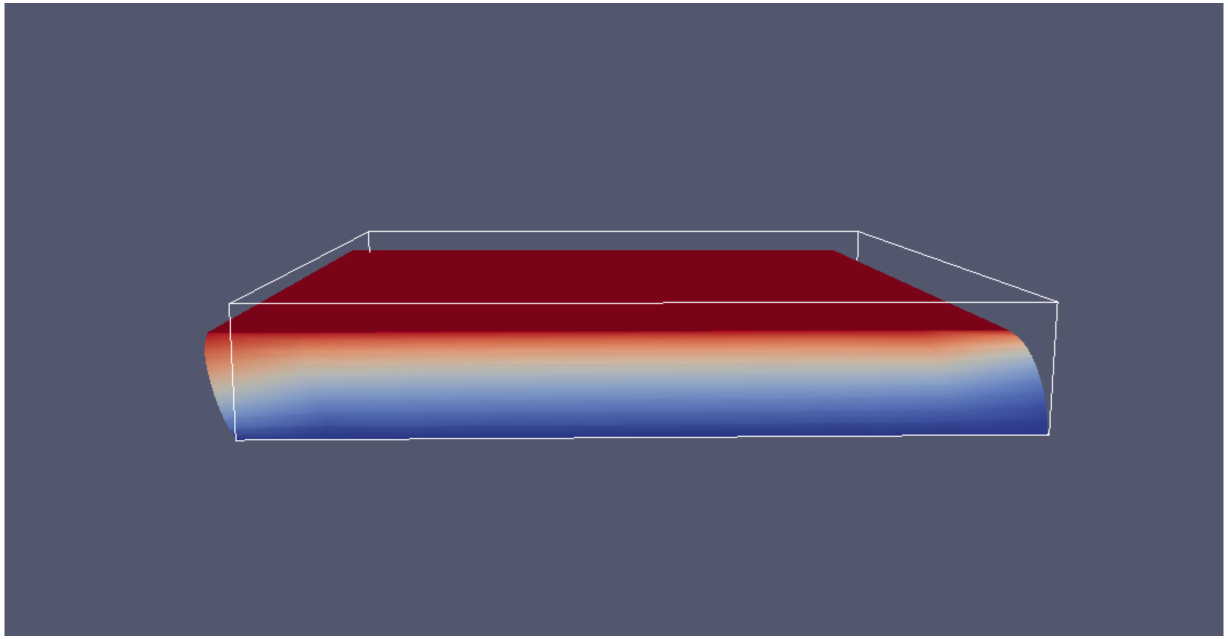
Balance of mass	$\dot{\rho}+\rho\,\mathrm{div}\,\boldsymbol{v}=0$
Balance of linear momentum	$\rho\dot{v}=\mathrm{div}\,\boldsymbol{v}+\rho\boldsymbol{b}+\rho\boldsymbol{b}^e$
Balance of angular momentum	$\overset{axial}{\boldsymbol{t}}\;\mathrm{skew}[\boldsymbol{\sigma}_C]=\rho\boldsymbol{c}$
Balance of energy	$\rho\dot{e}=\boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}}+\rho r+\rho r^e-\mathrm{div}\,\boldsymbol{q}$

$\rightarrow$ The new introduced terms $\boldsymbol{b}^e,\boldsymbol{c}$ and r^e have connections with electrical potential ϕ and polarization field $\boldsymbol{p}$.

$\rightarrow$ These quantities should be recognized in the next step.

5. Summary and conclusions

Deformation of solid electrolyte due to direction in 3-D is explicitly implemented and illustrated:



Results obtained

- Directional effect of the newly-discovered solid electrolyte is modeled by coordinate-free tensor structure (First approach).
  → A thermodynamic consistent formulation is presented..
- The coupling effect of polarization and deformation is illustrated by electro-elastic coupled problem based on continuum physics (Second approach).
  → Loss of symmetry in the stress tensor of the coupling two-field problem is proved.
- Numerical 1D-2D-3D implementation based on open source is accomplished and ready to deliver and easy to develop.
  → Accessible via Gitlab: https://git.rwth-aachen.de/tuan.vo/dealii-llzo

5. Summary and conclusions

On-going and future research directions

- Time-dependent implementation + Numerical analysis + Validations + Verification.
- Continue developing and bringing the coupled electro-elastic problem to an end (Second approach).
- Combine electro-elastic coupling + coordinate-free structural tensor problem, when possible.
- Bridging scale into quantum physics: Update information from quantum for continuum.
- Dendrite formation: transport problem.