Outlook
Complex multiphysics/multiscale applications with 4C – Current research projects

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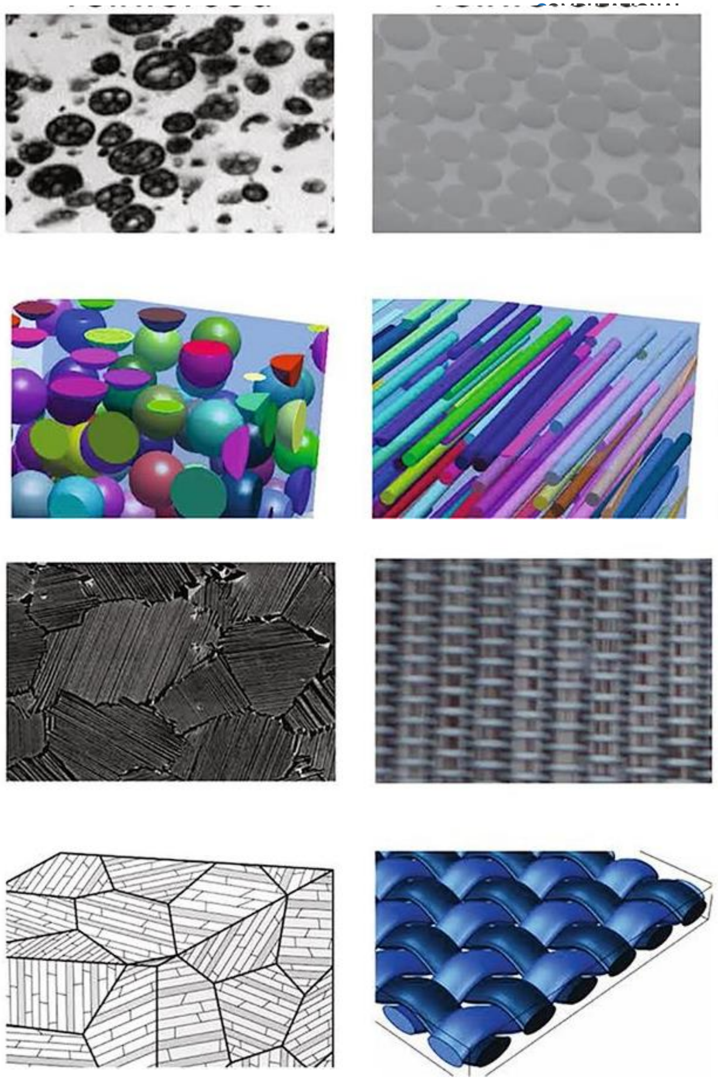
Brief outlook into current applications with 4C Multiphysics

- **Multiscale example**
- Battery example
- Biomechanics examples
  - Lung
  - Shoulder

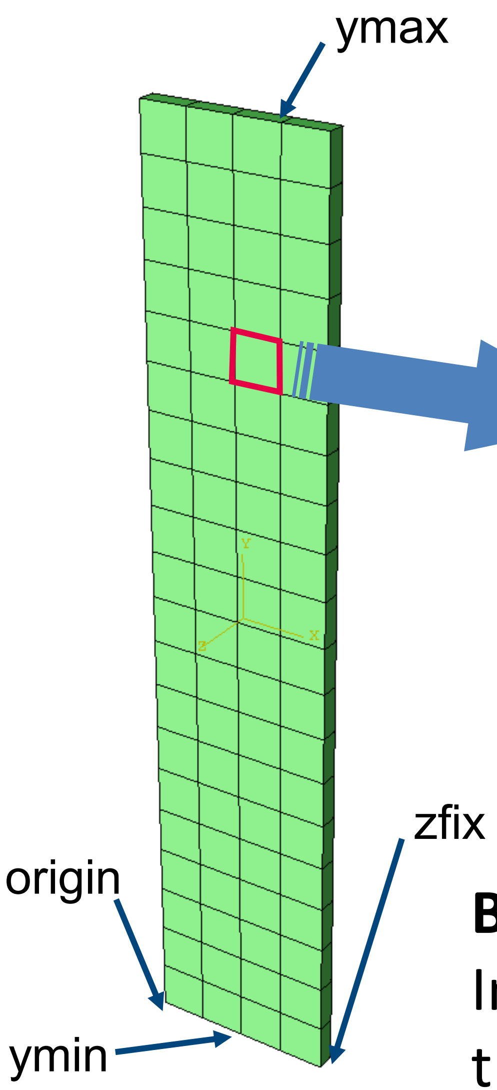
Multiscale: Models with microstructure

- Microstructures of materials may be complex
  - Fiber or particle reinforced composites, woven fabrics materials
  - Metals with differently oriented grains, grain boundaries
  - Structured materials with microstructural lattices
- Assumption: Characteristic length of microstructure << main problem
  - Microstructure presumed as a repeated unit cell
  - Single unit cell can be modeled easily

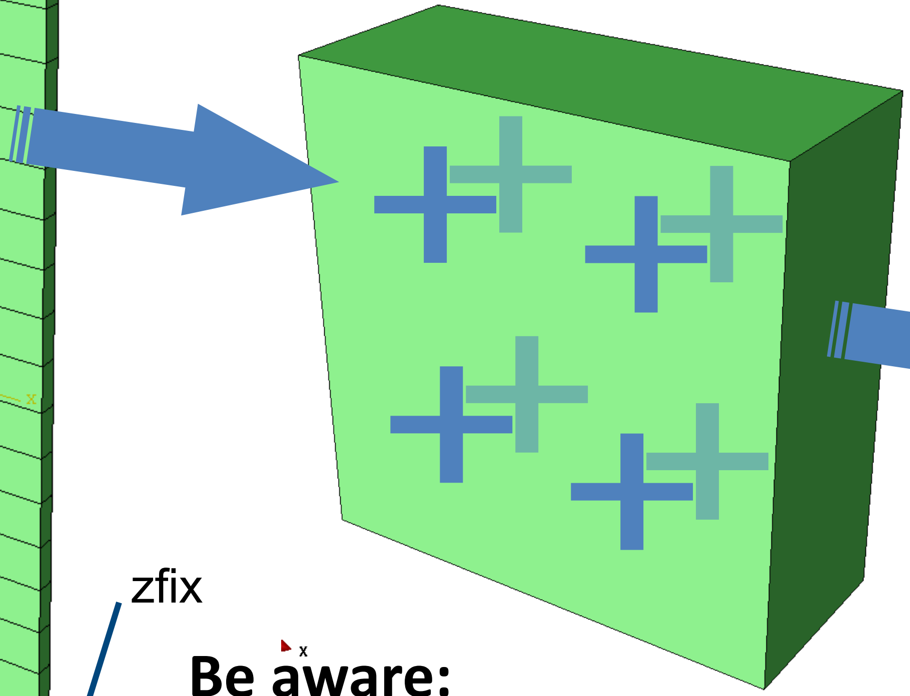


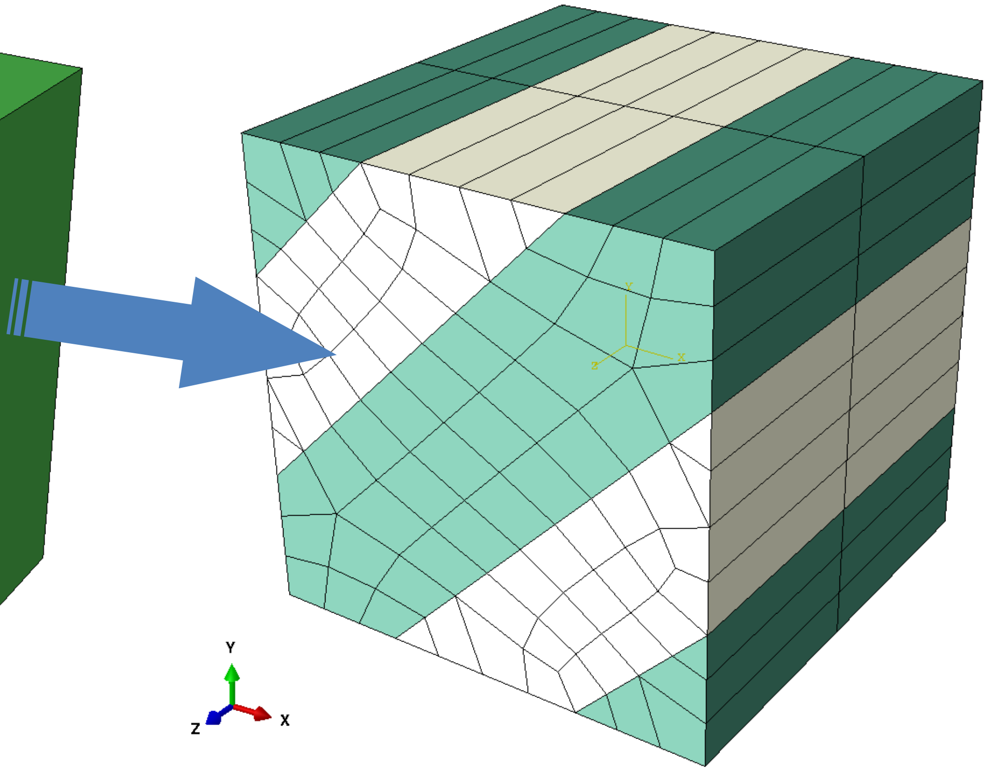
Bargmann, S. et al. (2018). *Progress in materials science*, *96*, 322-384, Fig. 2

Multiscale: Micro-macro coupling in 4C



Macro structure (here: tensile bar) contains in each Gauss Point a (here: lamellar) microstructure





Be aware:

Instead of 80 Elements,

the model solves now 80 x 8 x 176 = 112.640 elements

Multiscale: Micro-macro coupling in 4C

What is needed?

- **An input file for the macroscopic structure (e.g.: tensile-macro.4C.yaml)**
  - New feature: Material definition is not given by a material model, but by a second input file representing the microstructure
- **Input file for the microstructure (e.g.: tensile-micro.4C.yaml)**
  - Contains conventional material models (elasticity, plasticity, etc.)
  - No Dirichlet or Neumann boundary conditions
  - Instead: Surface definition for applying the deformation gradient of the macro-structure element Gauss Point
  - Definition of an additional solver for static homogenization

Multiscale: Micro-macro coupling in 4C

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Necessary modifications…

… on the macro-file (tensile-macro.4C.yaml)

- New material: MAT_Struct_Multiscale
- Boundary conditions:
  Hold at the bottom, pull at the top, some fixture

```yaml
MATERIALS:
  - MAT: 1
    MAT_Struct_Multiscale:
      MICROFILE: "tensile-micro.4C.yaml"
      MICRODIS_NUM: 1
```

… on the microstructure (tensile-micro.4C.yaml)

- Surface definition for applying the deformation gradient of the macro-structure element Gauss Point

```yaml
MICROSCALE CONDITIONS:
  - E: 1
    ENTITY_TYPE: node_set_id
  - E: 2
    ENTITY_TYPE: node_set_id
  - E: 3
    ENTITY_TYPE: node_set_id
  - E: 4
    ENTITY_TYPE: node_set_id
  - E: 5
    ENTITY_TYPE: node_set_id
  - E: 6
    ENTITY_TYPE: node_set_id
```

Multiscale: Micro-macro coupling in 4C

Run the simulation in an MPI environment:

```
mpirun -np 4 4C tensile-macro.4C.yaml results/tensile
```

Note: With this command,

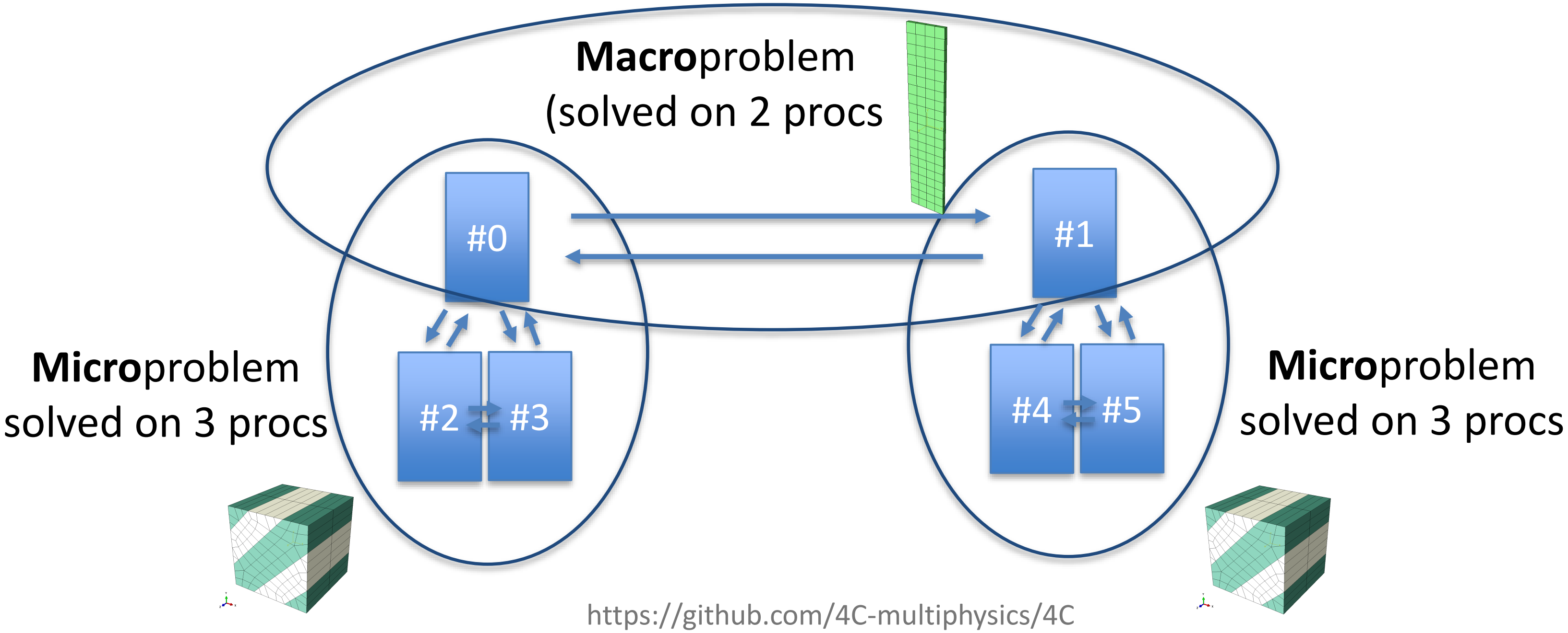
- the macrostructure is simulated on all (here: 4) CPUs
- each microstructure runs on a single CPU (equivalent to a conventional material model)
- all material points, i.e., microstructures, are run sequentially for each block within the macrostructure

Multiscale: Micro-macro coupling in 4C

Alternative:

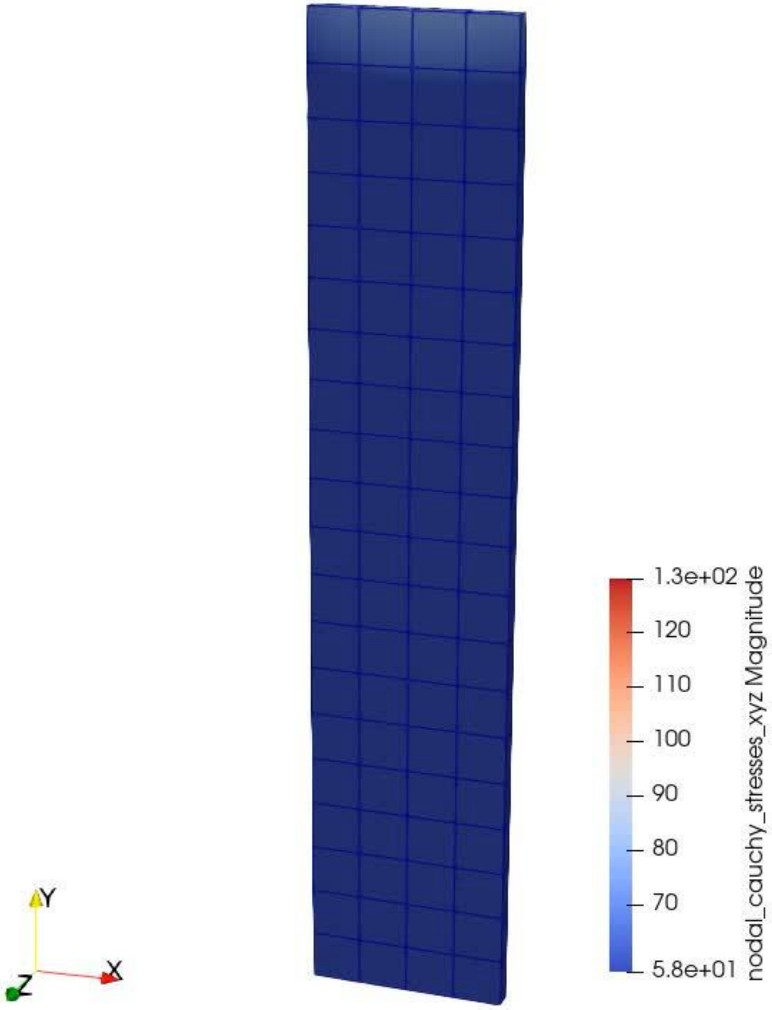
- If one had more cores, one might use additional cores for the microstructure

```
mpirun -np 6 4C -nptype=separateInputFiles -ngroup=2 -glayout=2,4 \
tensile-macro.4C.yaml tensile multiscale_npsupport.4C.yaml dummy
```

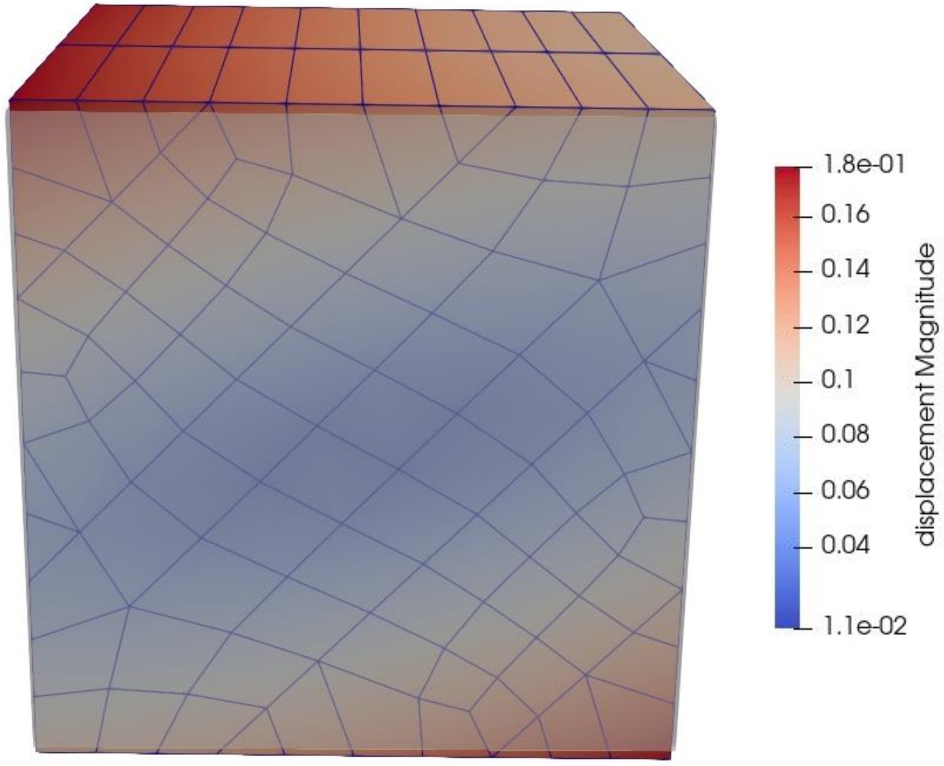


Multiscale: Micro-macro coupling in 4C

Results



Microstructure:
Displacement in Macro-element 47 at last step



Brief outlook into current applications with 4C Multiphysics

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- **Battery example**
- Biomechanics examples
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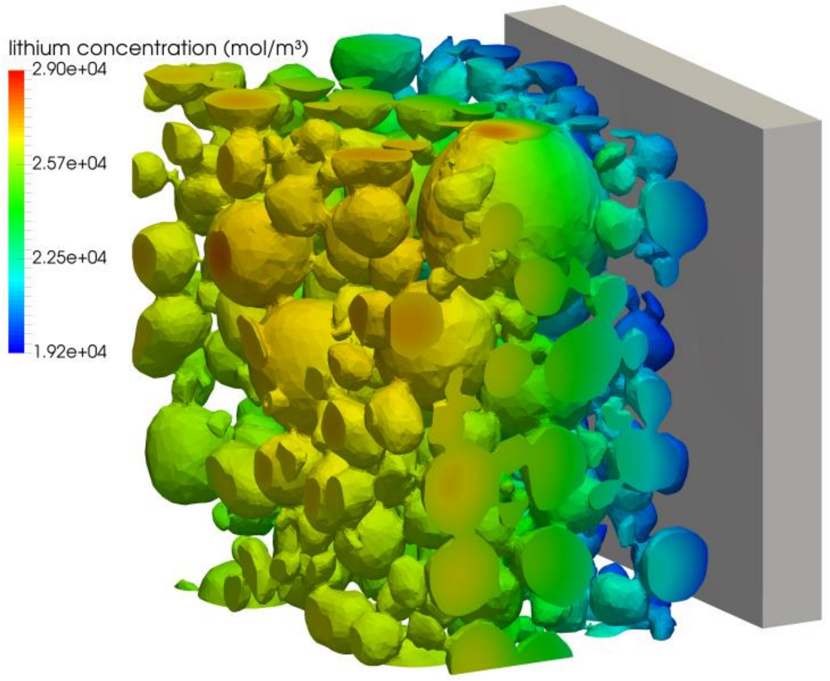
Physics-based battery simulations

Physics-based simulation

- More detailed understanding of the underlying physical and chemical processes
- Prediction of battery cell behavior under operational and extreme conditions
- Aid in design of new materials and cells

Challenges

- Complex microstructural geometries
- Consideration of multiple physical fields:
  - Solid mechanics field
  - Electrochemical field
  - Thermal field
- Strong interaction between the fields → coupled multiphysics problem
- Multitude of model parameters → uncertainty



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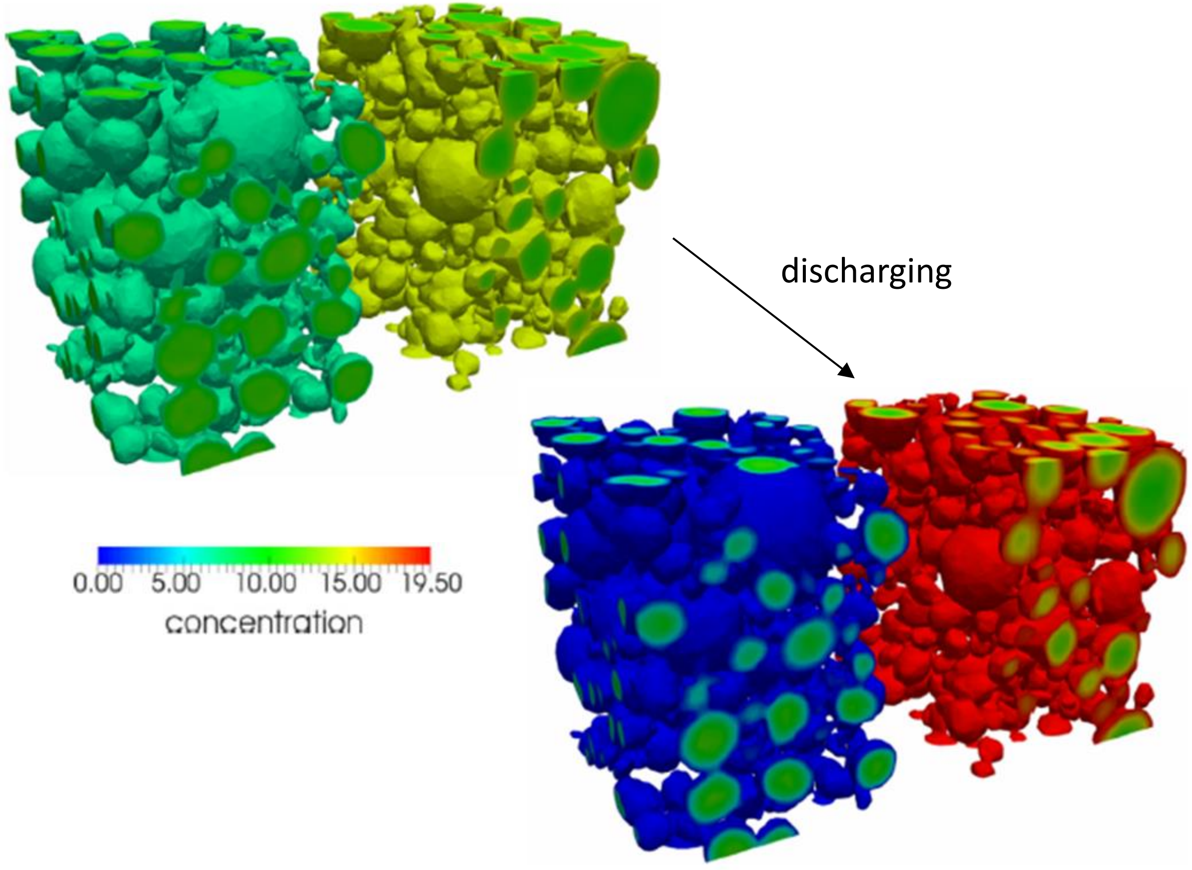
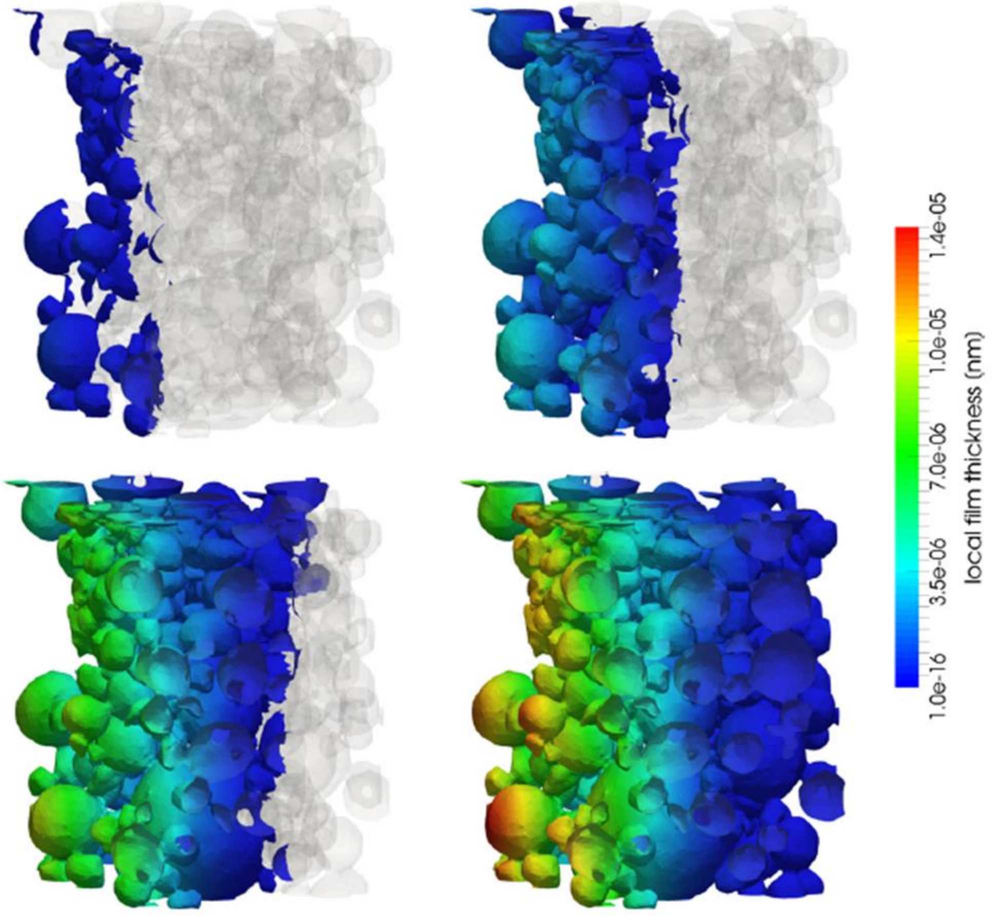
Spotlights on Lithium-ion battery research

Microstructure-Resolved Scalar-Transport-Electro-Thermo Interaction



Fang et al 2019 Comput. Methods Appl. Mech. Eng. 350 803-835; DOI: 10.1016/j.cma.2019.03.017

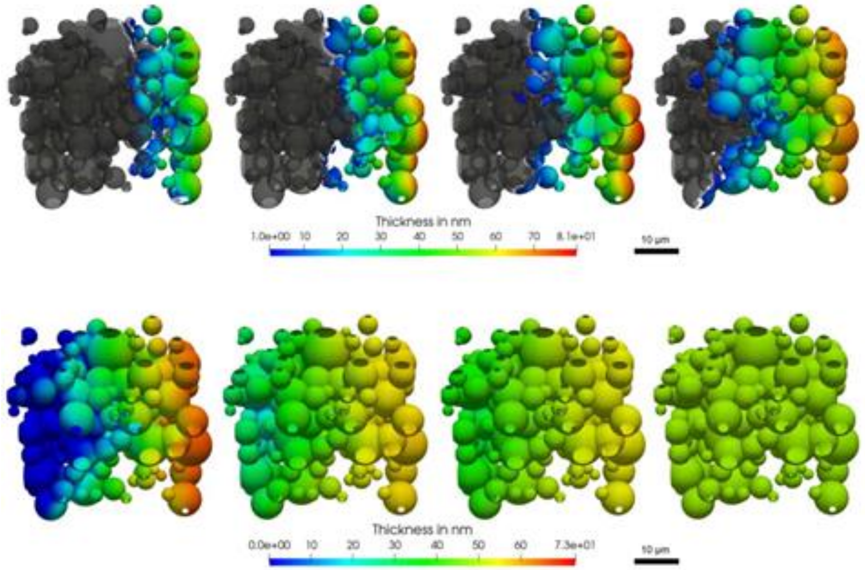
Lithium Plating and Stripping

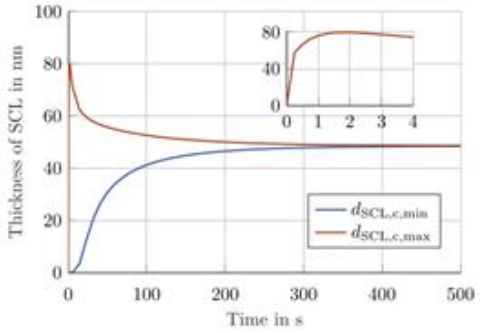


Fang et al 2022 J. Comput. Phys. 461 111179; DOI: 10.1016/j.jcp.2022.111179

Complex interface phenomena in solid-state batteries

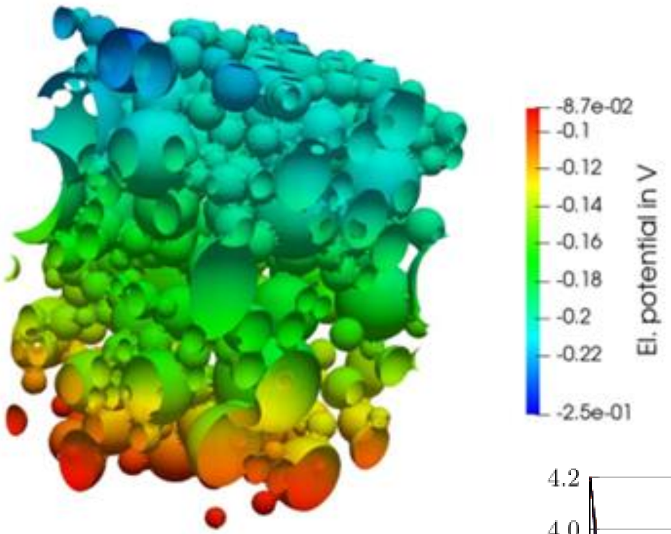
Space charge layers

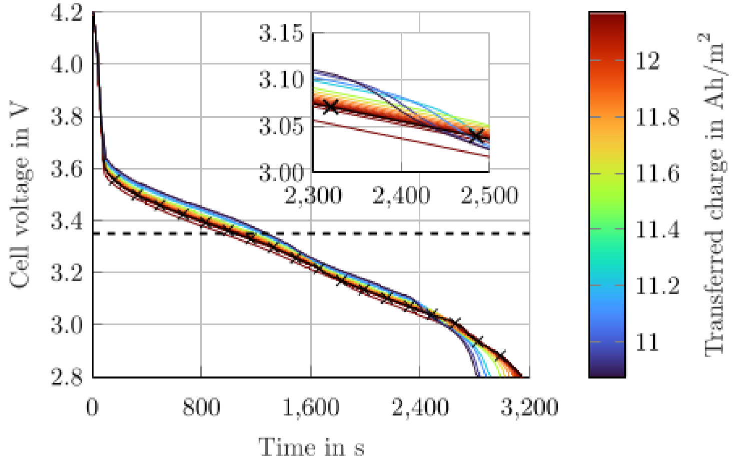




Sinzig et al 2023 J. Electrochem. Soc. 170 040513; DOI: 10.1149/1945-7111/acc692

Coating layers

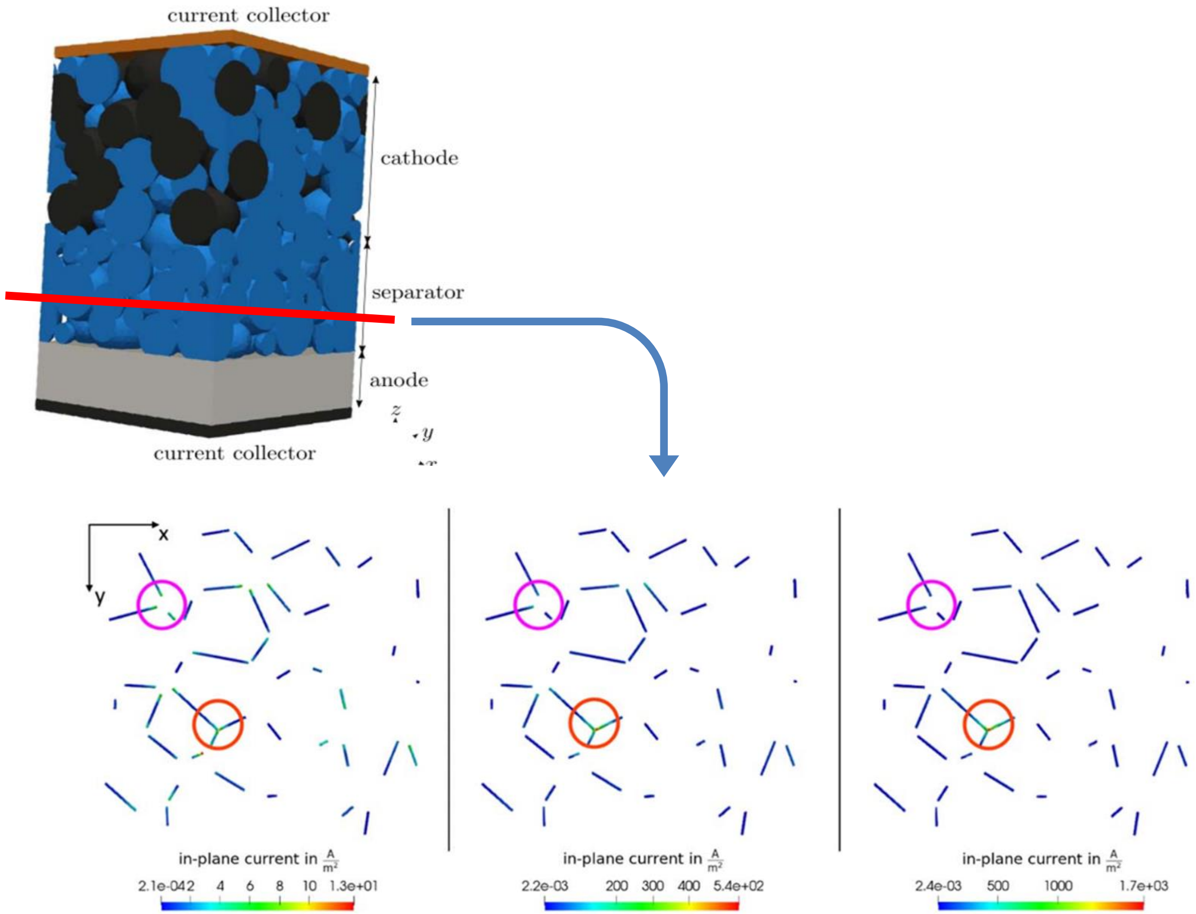




Sinzig et al 2023 J. Electrochem. Soc. 170 100532; DOI: 10.1149/1945-7111/ad0264

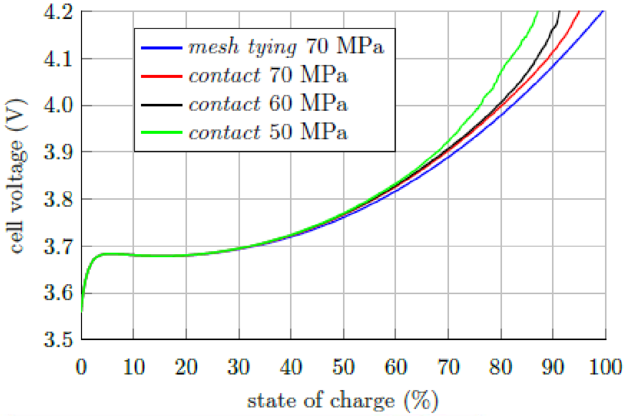
Complex interface phenomena in solid-state batteries

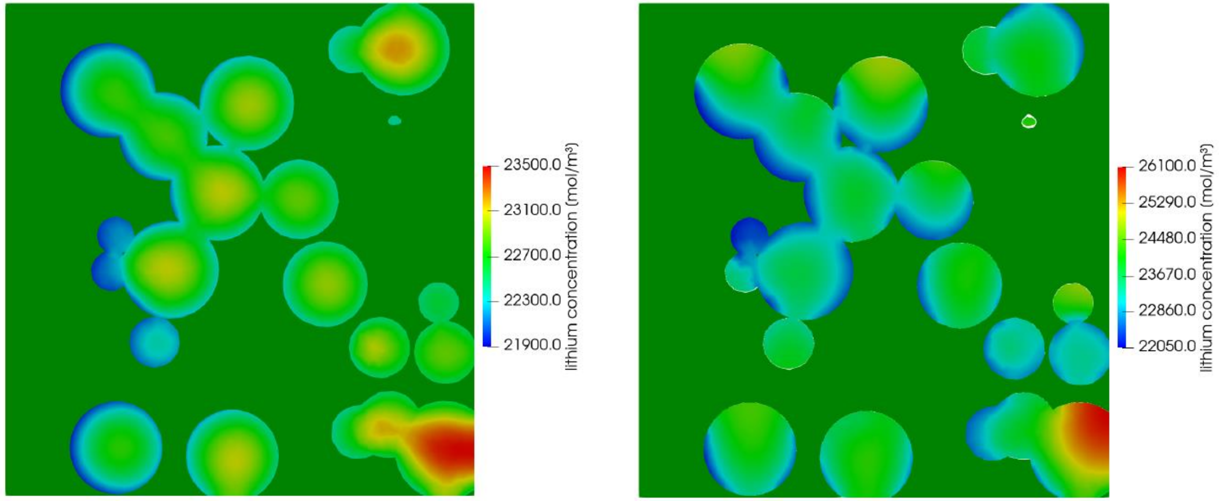
Grain boundary transport



Sinzig et al 2024 J. Electrochem. Soc. 171 040505; DOI: 10.1149/1945-7111/ad36e4

Delamination of active material and solid electrolyte





Schmidt et al 2024 J. Electrochem. Soc. 171 100502; DOI: 10.1149/1945-7111/ad76dc

Input file for battery simulation (excerpt)

There is a bunch of nice methods available but there is no free lunch ;-)

→ How to setup grain boundary transport in the input file for a solid-state battery

- Geometry file including node set definitions of surfaces that shall be treated as grain boundaries

```
SSI CONTROL/MANIFOLD:
  ADD_MANIFOLD: true
  INITIALFIELD: field_by_condition
  INITFUNCNO: 5
  LINEAR_SOLVER: 1
  OUTPUT_INFLOW: true
```

General manifold settings

```
DESIGN SURF SCATRA MANIFOLD INITIAL FIELD CONDITIONS:
  - E: 3
    FIELD: ScaTra
    FUNCT: 5
  - E: 4
    FIELD: ScaTra
    FUNCT: 6
```

```
FUNCT5:
  - COMPONENT: 0
    SYMBOLIC_FUNCTION_OF_SPACE_TIME: "2.0+(x-0.001)/0.002"
  - COMPONENT: 1
    SYMBOLIC_FUNCTION_OF_SPACE_TIME: "1.0"
FUNCT6:
  - COMPONENT: 0
    SYMBOLIC_FUNCTION_OF_SPACE_TIME: "2.0+(x+0.001)/0.002"
  - COMPONENT: 1
    SYMBOLIC_FUNCTION_OF_SPACE_TIME: "1.0"
```

ScaTra field always has two degrees of freedom per node (mass & charge), thus 2 components must be defined

```
DESIGN SSI MANIFOLD SURF CONDITIONS:
  - E: 3
    ConditionID: 1
    ImplType: ElchDiffCond
    thickness: 1
  - E: 4
    ConditionID: 2
    ImplType: ElchDiffCond
    thickness: 1
```

Create manifolds for surfaces defined by node sets 3 and 4

```
DESIGN SSI MANIFOLD KINETICS SURF CONDITIONS:
  - E: 3
    ConditionID: 1
    ManifoldConditionID: 1
    KINETIC_MODEL: ConstantInterfaceResistance
    ONOFF: [1, 1]
    RESISTANCE: 0.0010364273109887785
    E-: 1
  - E: 4
    ConditionID: 2
    ManifoldConditionID: 2
    KINETIC_MODEL: ConstantInterfaceResistance
    ONOFF: [1, 1]
    RESISTANCE: 0.00010364273109887784
    E-: 1
```

Definition of the kinetics between the grain boundary (modeled as manifold) and the surrounding bulk material

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- **Biomechanics examples**
  - **Lung**
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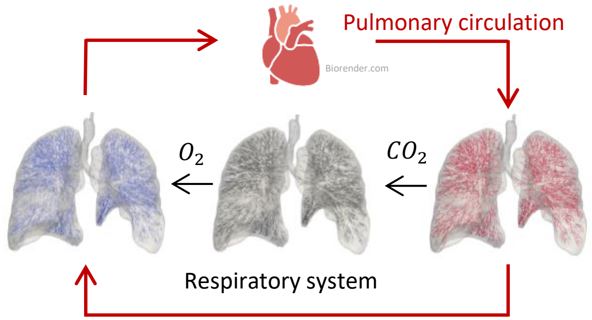
A mixed-dimensional approach for modeling the respiratory and circulatory system of the human lungs using porous media

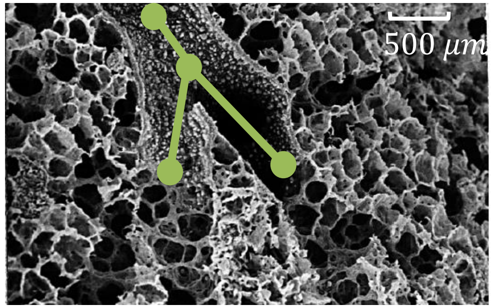
Objective: Physically based, predictive and patient-specific computational lung model

→ Capture complex effects in respiratory zone (like inter-alveolar connectivity)
→ Coupling respiratory system and pulmonary circulation
→ Modeling gas exchange
→ Add additional phases (like lung water)

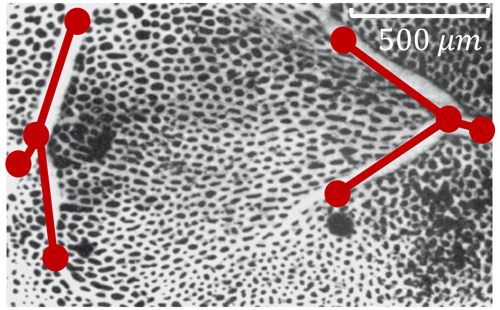


Modelling approach:

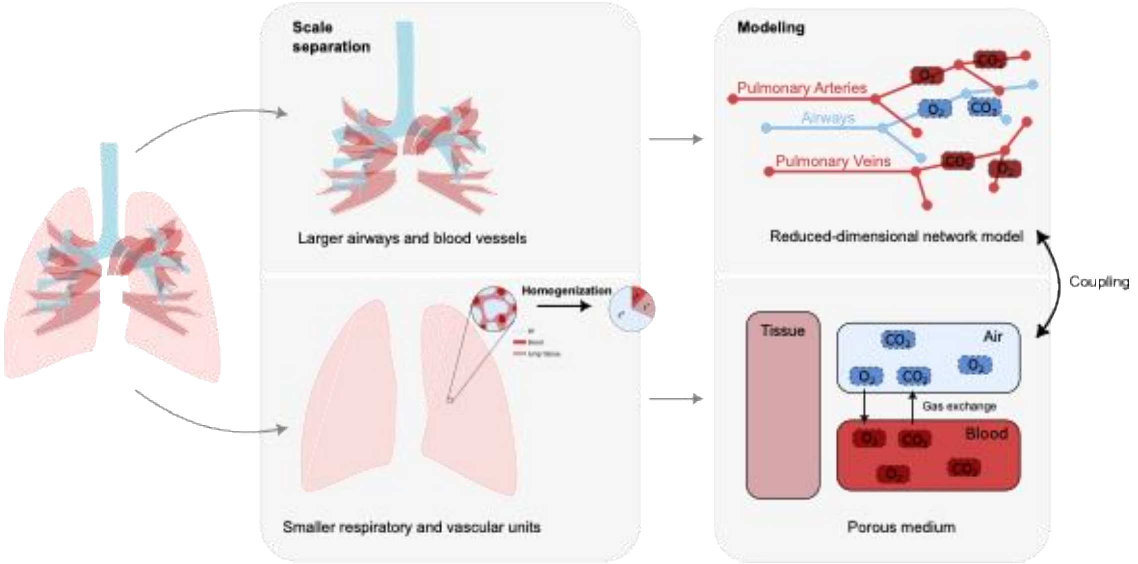
→ Smaller airways and blood vessels: **porous medium**
→ Larger airways and blood vessels: **discrete 0D networks**



L. Berger et al. "A poroelastic model coupled to a fluid network with applications in lung modelling". (2016)

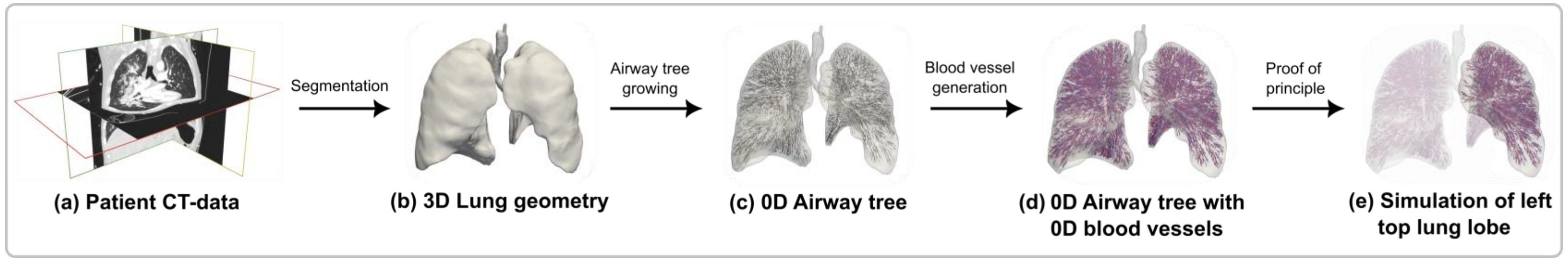


J. B. West and A. M. Luks. West's respiratory physiology: the essentials. Tenth edition.(2016)



A mixed-dimensional approach for modeling the respiratory and circulatory system of the human lungs using porous media

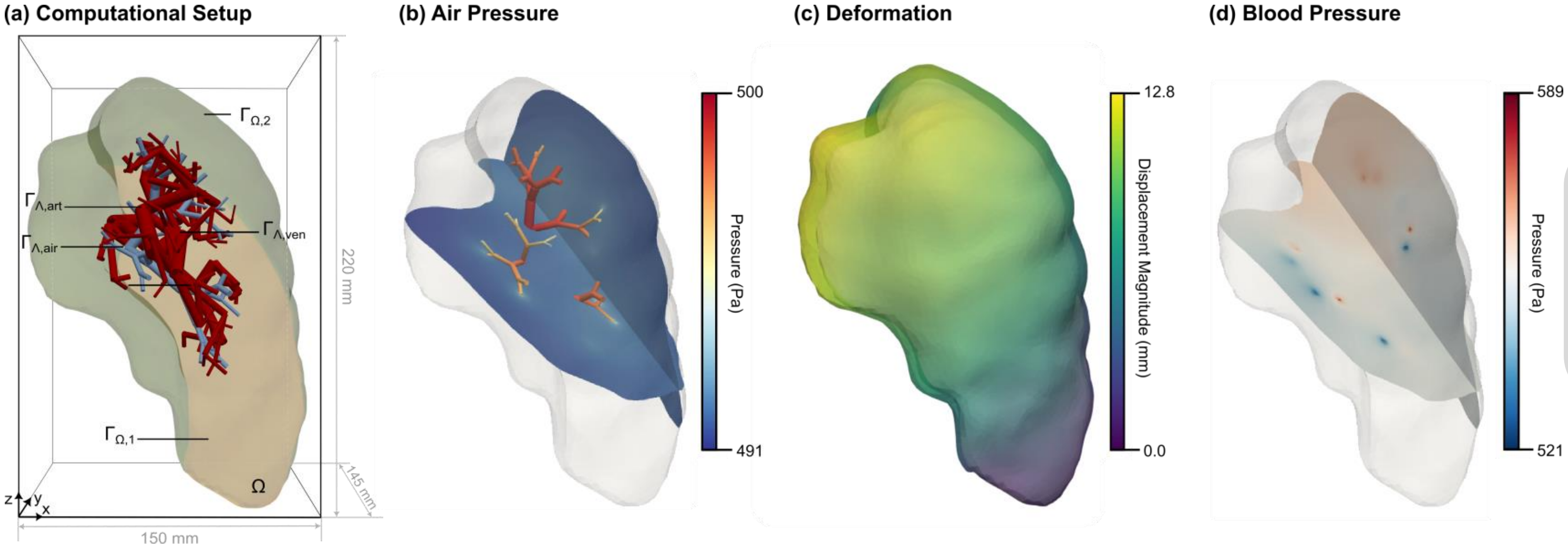
Workflow for patient-specific geometry generation



Ismail M. (2014), Ismail M et al. (2013). doi: 10.1002/cnm.2577

(b) segment the lung lobes and visible first airway generations
(c) algorithms to generate the peripheral larger airway branches
(d) generate the larger pulmonary blood vessels

Simulation results



- Simulation of one breathing cycle (5 sec.)
- Geometry of left top lung lobe including five generations of discretely modeled larger airways, arteries, and veins
- Results are shown at end-inspiration

Köglmeier et al, Coupled mixed-dimensional multiphase porous media approach for modeling airflow, blood flow, and gas exchange in the human lungs, in preparation

Brief outlook into current applications with 4C Multiphysics

- Multiscale example
- Battery example
- **Biomechanics examples**
  - Lung
  - **Shoulder**

Shoulder physiology: Computational biomechanics to address clinical challenges

Mobility

<u>Most flexible</u> joint in the human body due to

- Anatomical structure of glenohumeral joint
- Complex muscular interactions

Stability

Dependent on surrounding <u>soft tissues</u>

- *Static* stabilizers: Ligaments, tendons, labrum
- *Dynamic* stabilizers: Active and passive muscles

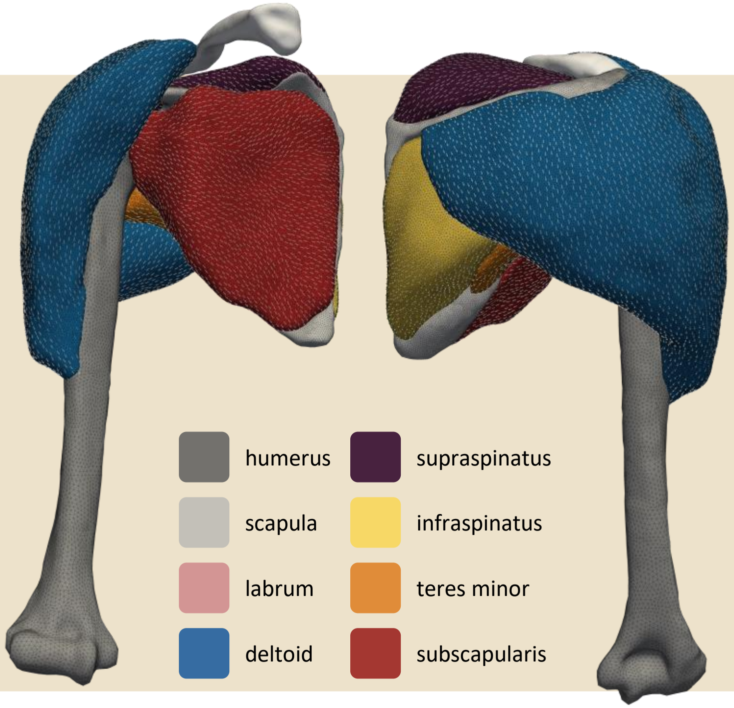
Dysfunction and injury is common and can have multiple causes
Challenges in clinical practice: diagnosis, treatment and monitoring

3D continuum-mechanical model

Constitutive models

Muscle-tendon complexes: Mixture model with muscle and tendon constituents

- Muscle: Generalized active strain model with spatiotemporally varying activation
- Tendon: Transversely isotropic model
- Bone, Labrum: St.-Venant Kirchhoff model



Boundary conditions

Tied constraints

- Muscles-bones (some regions)

Contact constraints

- Bone-bone
- Muscle-bone
- Muscle-muscle

Geometry and mesh

- Patient-specific geometry
- Segmented from real imaging data
- Quadratic tets with F-bar technology

Input file for shoulder simulation (excerpt)

```
MATERIALS:
- MAT: 1
  MAT_Mixture:
    MATIDMIXTURERULE: 11
    MATIDSCONST: [22, 33]
```

A mixture material model consisting of two constituents: **Muscle** and **tendon**

```
- MAT: 11
  MIX_Rule_Simple:
    DENS: 0.1
    MASSFRAC:
      from_file: "muscle_tendon_massfractions.json"
```

Constituents are mixed according to the element-wise defined mass fractions

```
{
    "MASSFRAC": {
        "62275": [
            0.8034154787554213,
            0.1965845212445787
        ],
        "62276": [
            0.9656991964185757,
            0.03430080358142429
        ],
        "62277": [
            0.9874255405171426,
            0.012574459482857403
        ],
        "62278": [
            0.9949756435926256,
            0.005024356407374442
        ],
```

Definition of mass fraction in an external json file

```
- MAT: 22
  MIX_Constituent_SolidMaterial:
    MATID: 222
- MAT: 222
  MAT_Muscle_Combo:
    ALPHA: 2.3795702114103094
    BETA: 0.5161005889693708
    DENS: 1e-06
    GAMMA: 27.107421574113225
    KAPPA: 10
    LAMBDAMIN: 0.5679564851414783
    LAMBDAOPT: 1.1806202453751011
    OMEGA0: 0.6388151301347268
    POPT:  64.68091032816055
    ACTIVATION_VALUES:
      from_file: "muscle_activations.json"
```

Active **muscle** material constituent with element-wise defined activation values

```
{
    "ACTIVATION_VALUES": {
        "62275": [[0.0, 0.0], [0.01, 0.123143], [0.02, 0.234234], [0.03, 0.345345]],
        "62276": [[0.0, 0.0], [0.01, 0.223143], [0.02, 0.334234], [0.03, 0.445345]],
        "62277": [[0.0, 0.0], [0.01, 0.675884], [0.02, 0.432423], [0.03, 0.532432]],
        "62278": [[0.0, 0.0], [0.01, 0.794304], [0.02, 0.543543], [0.03, 0.645345]],
```

Definition of time-activation value pairs in an external json file

```
- MAT: 2
  MAT_Struct_StVenantKirchhoff:
    YOUNG: 3e7
    DENS: 0.13
    NUE: 0.3
- MAT: 3
  ...
```

Further material model definitions, e.g., bone, labrum, ligaments, ...

```
- MAT: 33
  ...
```

Tendon material constituent definition

Input file for shoulder simulation (excerpt)

```
CONTACT DYNAMIC:
  LINEAR_SOLVER: 2
  STRATEGY: Lagrange
  SYSTEM: Condensed
MORTAR COUPLING:
  ALGORITHM: Mortar
  LM_SHAPEFCN: Dual
  LM_QUAD: quad
  LM_DUAL_CONSISTENT: none
  SEARCH_ALGORITHM: BinaryTree
  SEARCH_PARAM: 0.5
  MESH_RELOCATION: None
```

Settings for contact and meshtying conditions

```
DESIGN SURF MORTAR COUPLING CONDITIONS 3D:
  - E: 45
    Initialization: Inactive
    InterfaceID: 1
    Side: Master
  - E: 2
    Initialization: Active
    InterfaceID: 1
    Side: Slave
  - E: 3
    Initialization: Inactive
    InterfaceID: 2
    Side: Master
  - E: 13
    Initialization: Active
    InterfaceID: 2
    Side: Slave
```

Tied interface 1 between surface 45 and 2

Tied interface 2 between surface 3 and 13

Tied constraints

```
DESIGN SURF MORTAR CONTACT CONDITIONS 3D:
  - E: 2
    Initialization: Inactive
    InterfaceID: 1
    Side: Master
  - E: 14
    Initialization: Inactive
    InterfaceID: 1
    Side: Slave
  - E: 4
    Initialization: Inactive
    InterfaceID: 2
    Side: Master
  - E: 5
    Initialization: Inactive
    InterfaceID: 2
    Side: Slave
```

Contact pair 1

Contact pair 2

Contact conditions

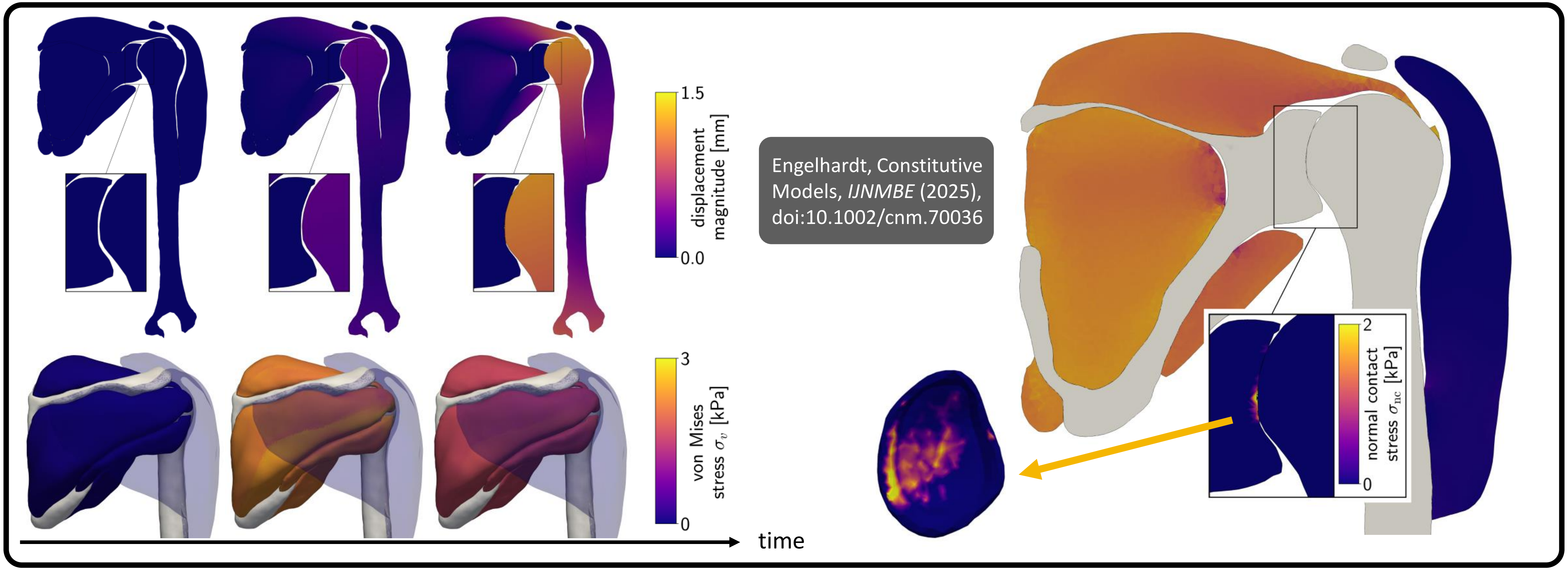
```
DESIGN SURF DIRICH CONDITIONS:
- E: 18
  NUMDOF: 3
  ONOFF: [ 1, 1, 1 ]
  VAL: [ 0, 0, 0 ]
  FUNCT: [ 0, 0, 0 ]
- E: 41
  NUMDOF: 3
  ONOFF: [ 1, 1, 1 ]
  VAL: [ 0, 0, 0 ]
  FUNCT: [ 0, 0, 0 ]
- E: 52
  NUMDOF: 3
  ONOFF: [ 1, 1, 1 ]
  VAL: [ 0, 0, 0 ]
  FUNCT: [ 0, 0, 0 ]
```

Dirichlet boundary conditions

Dynamic stabilization of the shoulder joint through rotator cuff muscle contraction

Concavity compression effect
Activation of the rotator cuff muscles centers the humeral head in the glenoid fossa. The joint space closes, and compressive forces stabilize the joint.

Simulate rotator cuff muscle contraction
→ Assess effect of different (pathological) activation patterns
→ Quantify stabilizing forces and pressure distributions on the joint surfaces



Summary

- 4C Multiphysics solves challenging real-world applications
- Extensible modular C++ software structure
- Freely available under LPGL-3.0-or-later
- https://github.com/4C-multiphysics/4C
- Join the community ☺
  (photo from our this year's workshop July 29th – 31st, 2025)