OpenFCST: Fuel Cell Simulation Toolbox

M. Secanell[1] , A. Putz[2] , P. Wardlaw[1], V. Zingan[1] , M. Bhaiya[1], M. Moore[1], J. Zhou[1], C. Balen[1] and K. Domican[1]

[1] Energy Systems Design Lab (www.esdlab.mece.ualberta.ca)
Mechanical Engineering Department, University of Alberta
[2] Automotive Fuel Cell Cooperation Corp.

226th ECS Meeting, October 5, 2014
Cancun, Mexico

ESDL ENERGY SYSTEMS DESIGN LABORATORY

UNIVERSITY OF ALBERTA

Introduction

- Fuel cell operation involves a myriad of coupled physical process
  - Multi-component reactant gas transport
  - Charge transport: Proton and electron transport
  - Liquid water transport: Two-phase flow
  - Heat transport
  - Electrochemical reaction
- Fuel cell mathematical models must account for all these physical process simultaneously
  - Complex coupled problem
  - “Constantly evolving” models

Introduction

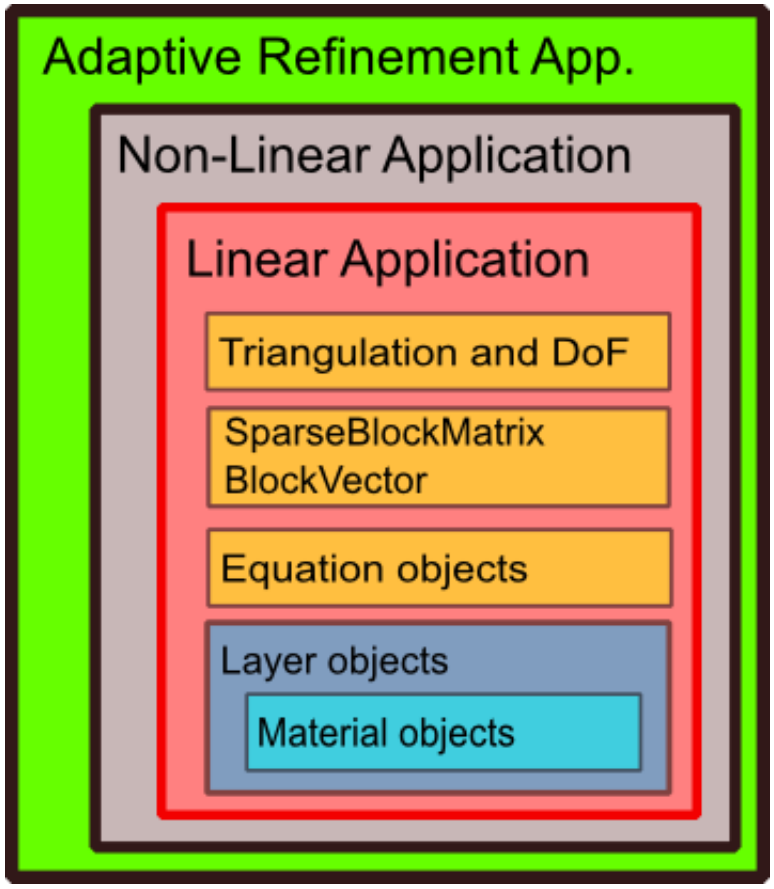
- There is a need to develop a collaborative fuel cell mathematical modeling software that can be shared and "evolved" within the fuel cell community
- The mathematical modeling software should be:
  - Multi-dimensional
  - Modular and easy to extend
    - New materials
    - New physics
  - Accessible to both users and mathematical model developers

What is OpenFCST?

- The Fuel Cell Simulation Toolbox (FCST) is an open-source mathematical modeling software for polymer electrolyte fuel cells
- It is a toolbox that contains:
  - **Pre-processors:** A fuel cell specific grid generator and a class to read meshes from an open-source mesh generator (we use SALOME, i.e. UNV)
  - **Solvers:** Multi-dimensional FEM solvers and nonlinear solvers as well as libraries of materials, layers and physical equations. FEM routines provided by the deal.II open-source libraries.
  - **Post-processors:** Functional evaluation algorithms and a VTK file generator (we use ParaView for post-processing)
  - **Design and optimization capabilities:** Parametric studies, parameter estimation and optimization algorithms. Optimization functionality provide by Dakota.

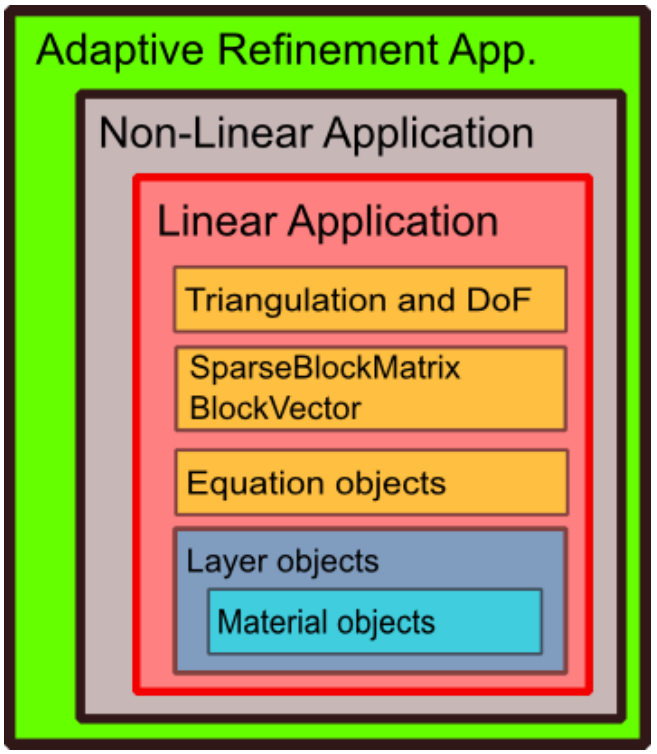
Main components of the code

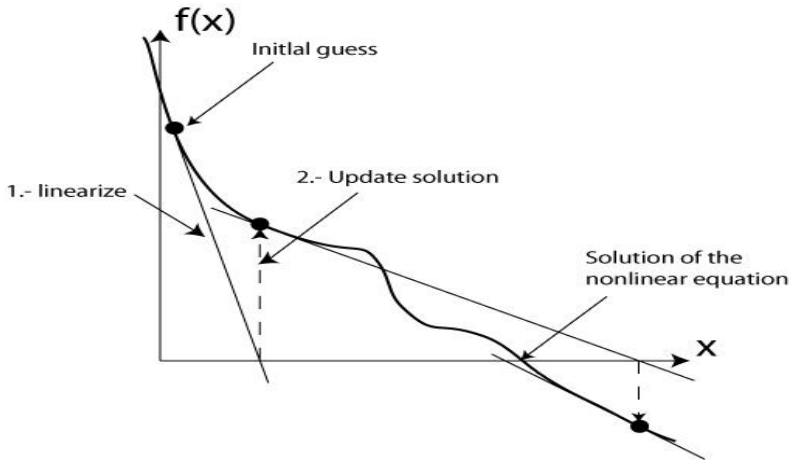
- Pre-processor
- Solver:
  - Application framework
  - Equation framework
  - Layer framework
  - Materials database
  - Reaction database
- Post-processor



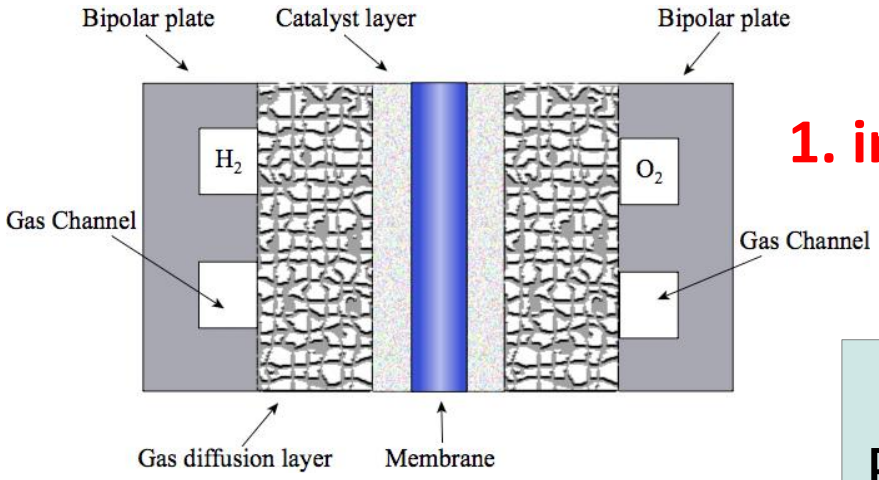
Application framework

- Two main applications
  - Linear finite element applications
    - Generate and store mesh
    - Read parameter file and initialize equation, layer and material objects
    - Loop over cells and assemble the FEM global matrix and right hand side
    - Solve the linear system
    - Applications developed: cathode, MEA and Laplace models
  - Wrapper applications
    - Implements iterative solution strategies for adaptive refinement, non-linear solvers and transient algorithms



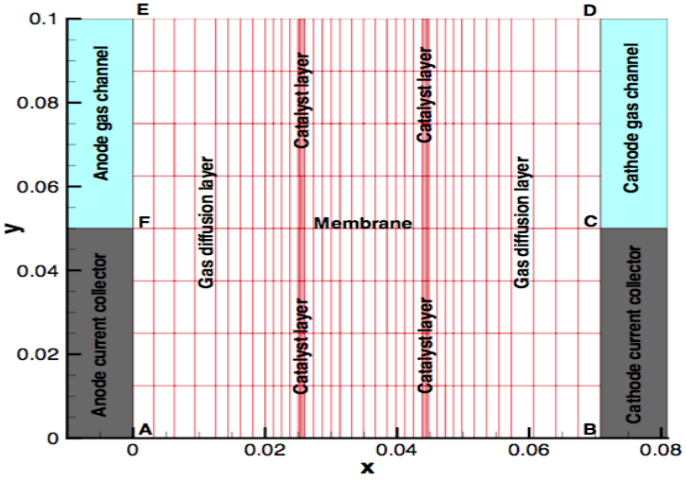


FEM application interface



1. initialize

FEM



$$
\left.
\begin{aligned}
\nabla \cdot (cD_{O_2}^{eff} \nabla x_{O_2}) &= S_{O_2} \\
\nabla \cdot (cD_{w}^{eff} \nabla x_{w}) &= S_w + S_\lambda \\
\nabla \cdot (\sigma_{m}^{eff} \nabla \phi_m) &= S_{H^+} \\
\nabla \cdot (\sigma_{S}^{eff} \nabla \phi_S) &= S_{e^-} \\
\nabla \left(n_d \frac{\sigma_m^{eff}}{F} \nabla \phi_m + \frac{\rho_{dry}}{EW} D_\lambda^{eff} \nabla \lambda \right) &= -S_\lambda
\end{aligned}
\right\}
$$

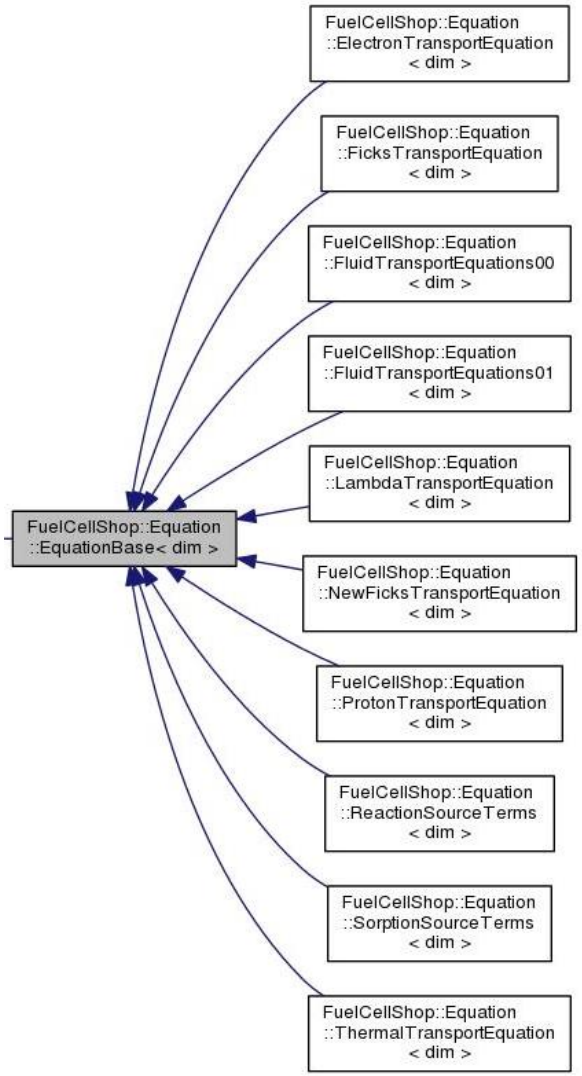
2. assemble

3. solve

$$
\begin{bmatrix} k_{11} & \dots & k_{1N} \\ \dots & k_{ii} & \dots \\ k_{N1} & \dots & k_{NN} \end{bmatrix} \begin{bmatrix} u_1 \\ \dots \\ u_N \end{bmatrix} = \begin{bmatrix} f_1 \\ \dots \\ f_N \end{bmatrix}
$$

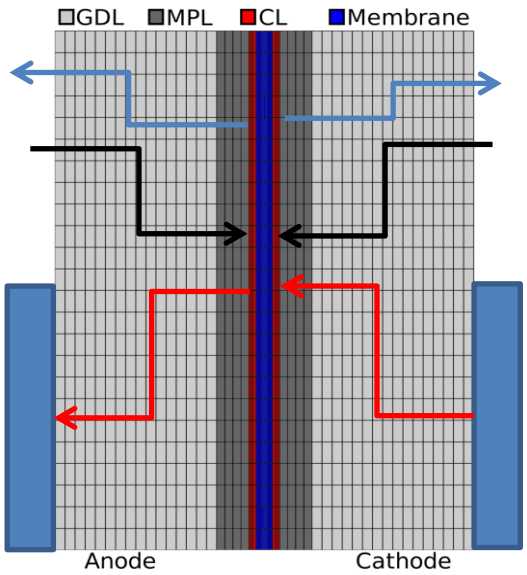
Equation framework

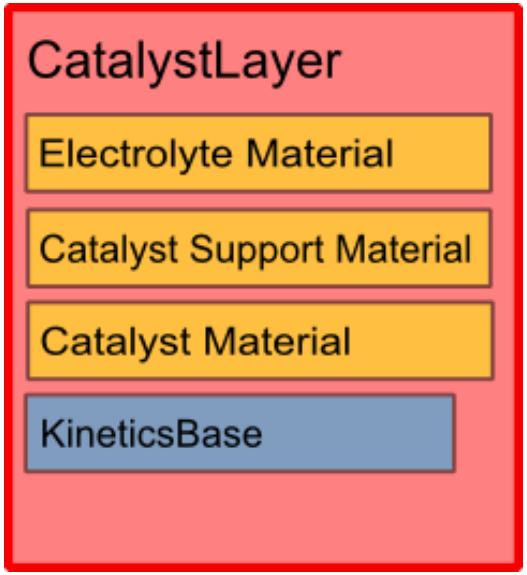
- Equation classes implement the weak form of the PDE that needs to be solved
- Currently implemented equations
  - Fick's law
  - Ohm's law
    - Electronic transport
    - Protonic transport
  - Water transport model
  - Reaction source term model
  - Thermal transport model (to be released this fall, openFCST 0.2)
  - Navier-Stokes equation model (not yet released)
  - Two-phase flow model – single equation (not yet released)



Layer framework

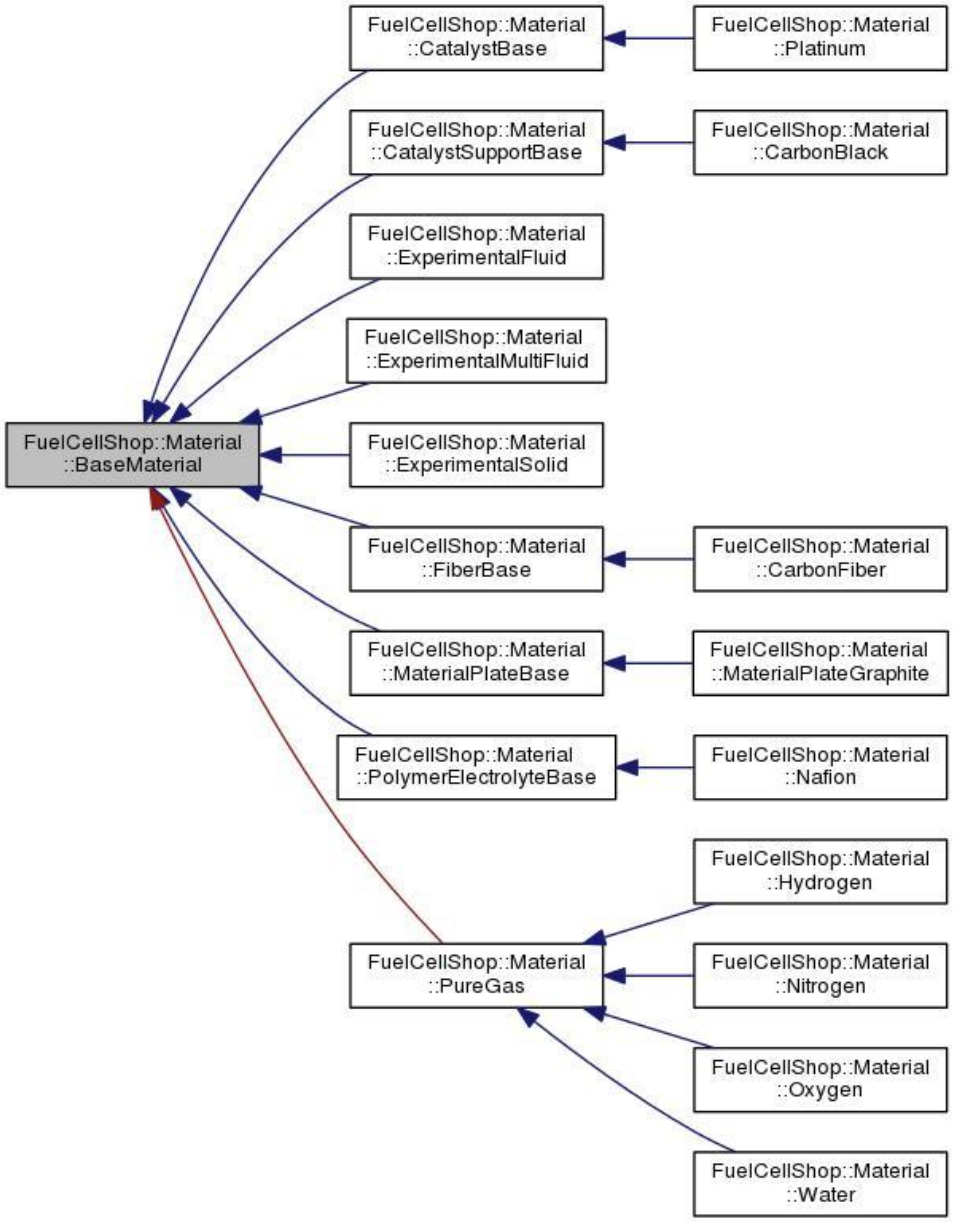
- Layer classes developed to compute
  - Effective transport properties
  - Derivatives of effective transport properties
  - Multi-scale integration requirements
- Materials objects inside layer to estimate the effective properties
- If the layer is reactive, kinetics object stored and used to compute reaction rates
- Layer interface allows users to swap layers via the input file





Material database

- Material database contains information on:
  - Gases: T_c, p_c, enthalpy, entropy, etc.
  - Catalysts: Activation energy, transfer coef., etc.
  - Catalyst supports
  - Fibers (for GDLs)
  - Electrolytes
- Materials of the same family can be swapped at real time



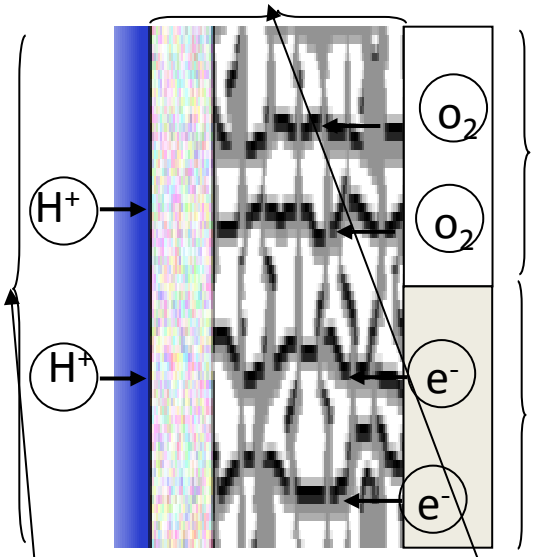
Kinetics database

- Fuel cell electrochemical reactions are complex, multi-step reactions involving many intermediates
  - To date, a detailed mathematical model does not exist
- An interface to explore novel kinetics has been developed
- Currently it contains:
  - A Tafel equation (simplest electrochemical reaction model)
  - A Butler-Volmer equation
  - A Double-trap multi-step kinetic model for the ORR
  - A Dual-path multi-step kinetic model for the HOR

Mathematical fuel cell model

- Steady-state and isothermal
- Solving for:
  - Oxygen mole fraction
  - Electrolyte potential
  - Solid potential
- Governing equation:

$$\nabla \cdot (c_{tot} D_{O_2}^{eff} \nabla x_{O_2}) - \frac{1}{4F} \nabla \cdot \vec{i} = 0$$
$$\nabla \cdot (\sigma_m^{eff} \nabla \phi_m) - \nabla \cdot \vec{i} = 0$$
$$\nabla \cdot (\sigma_S^{eff} \nabla \phi_S) + \nabla \cdot \vec{i} = 0$$

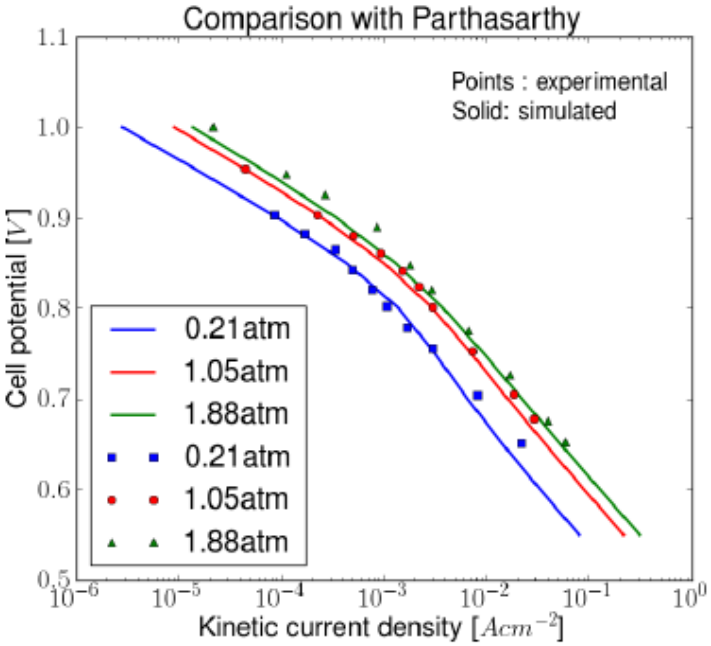


$$x_{O_2} = x_{O_2}^0$$
$$\vec{n} \cdot \nabla \phi_S = 0$$
$$\vec{n} \cdot \nabla \phi_m = 0$$
$$\vec{n} \cdot \nabla x_{O_2} = 0$$
$$\phi_S = 0$$
$$\vec{n} \cdot \nabla \phi_m = 0$$
$$\vec{n} \cdot \nabla x_{O_2} = 0$$
$$\vec{n} \cdot \nabla \phi_S = 0$$
$$\phi_m = \phi_0$$
$$\vec{n} \cdot \nabla x_{O_2} = 0$$
$$\vec{n} \cdot \nabla \phi_S = 0$$
$$\vec{n} \cdot \nabla \phi_m = 0$$

Mathematical model: Electrochemical reactions

- Tafel model usually used in fuel cells

$$\nabla \cdot \vec{i} = A_v i_0^{ref} \left(\frac{c_{O_2,g|l}}{c_{O_2}^{ref}} \right)^{\gamma} \exp\left(-\frac{\alpha_c F}{RT} (\phi_s - \phi_m) \right)$$



- ORR is a multi-step reaction

Dissociative adsorption (DA): $1/2O_2 \Leftrightarrow O_{ad}$
Reductive adsorption (RA): $1/2O_2 + H^+ + e^- \Leftrightarrow OH_{ad}$
Reductive transition (RT): $O_{ad} + H^+ + e^- \Leftrightarrow OH_{ad}$
Reductive desorption (RD): $OH_{ad} + H^+ + e^- \Leftrightarrow H_2O$

- The source term in the cathode is

$$\nabla \cdot i = j_k = j^* e^{\frac{-\Delta G^*_{RD}}{kT}} \theta_{OH} - j^* e^{\frac{-\Delta G^*_{-RD}}{kT}} (1 - \theta_O - \theta_{OH})$$

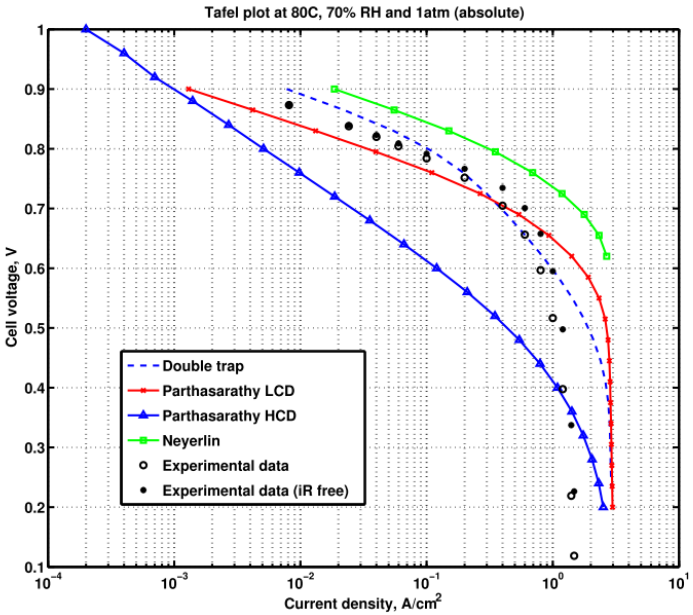
$$\Delta G^*_{RD} = \Delta G^{*0}_{RD} + \beta e \eta \qquad \Delta G^*_{-RD} = \Delta G^{*0}_{RD} + \Delta G^0_{OH} - \beta e \eta$$

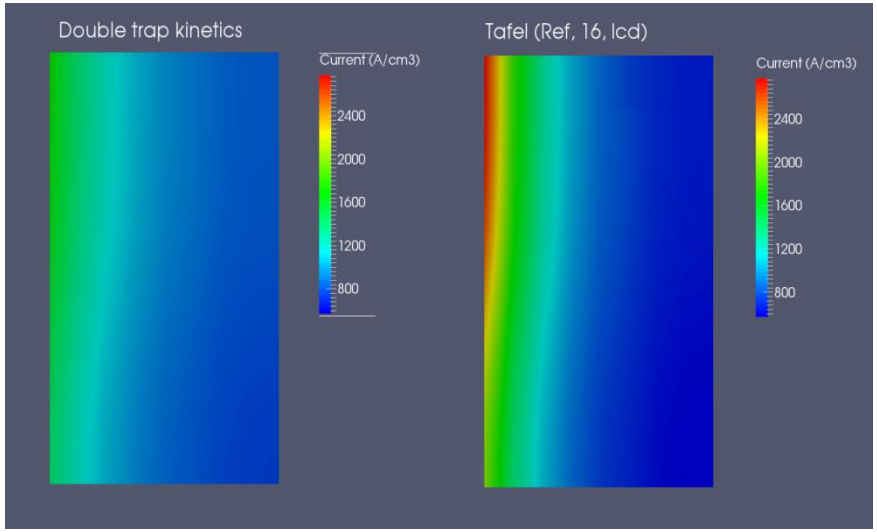
where $\eta = \phi_s - \phi_m - E_{eq}$

For more info: Moore et al., JES, 160(6): F670-F681, 2013

Mathematical model: Electrochemical reactions

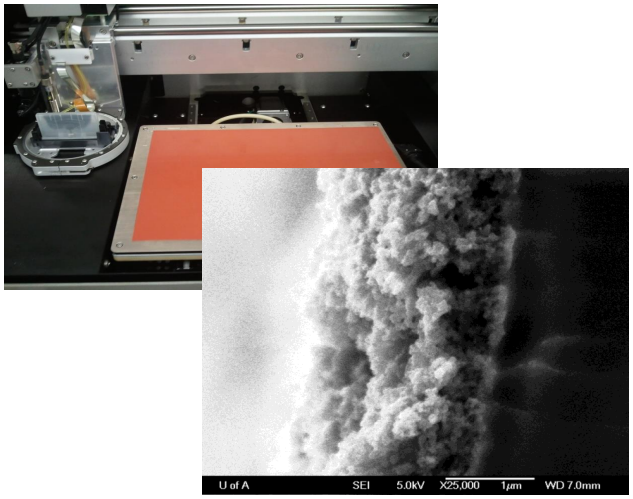
- Tafel plot shows the effect of the kinetic model
  - Doubling due to kinetics
  - Doubling due to mass
- Effect of kinetic model clearly visible in reaction rate distribution @1A/cm^2
  - Layer is less reactive, i.e. higher utilization

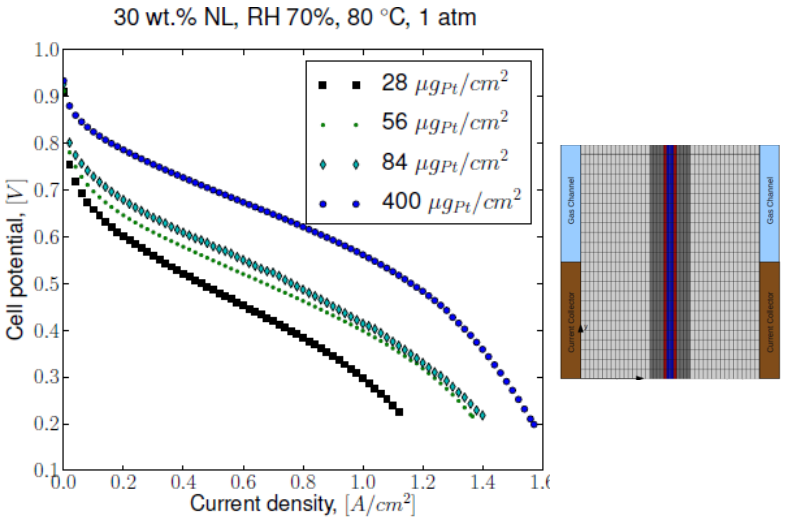


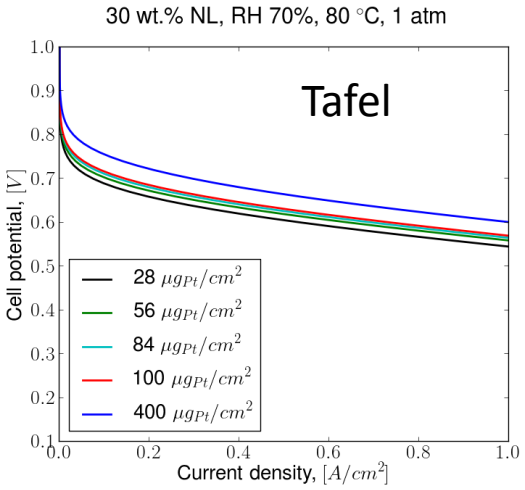


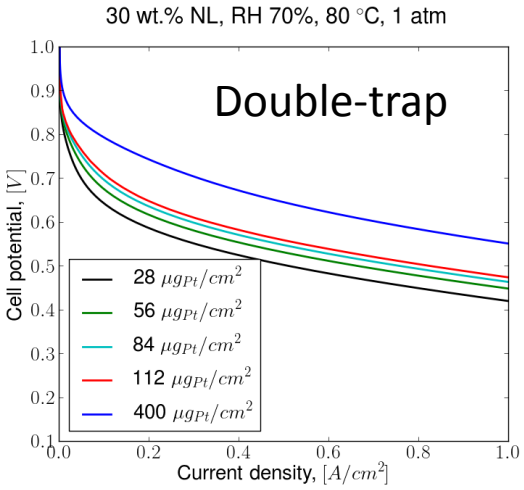
Mathematical model: Electrochemical reactions MEA model and experiments (80°C, 70%RH)

- Scale-up cathode model to full MEA simulation with micro-scale model
- MEA model based on Tafel over predicts performance for thin electrodes
- Double-trap model is able to predict voltage losses accurately



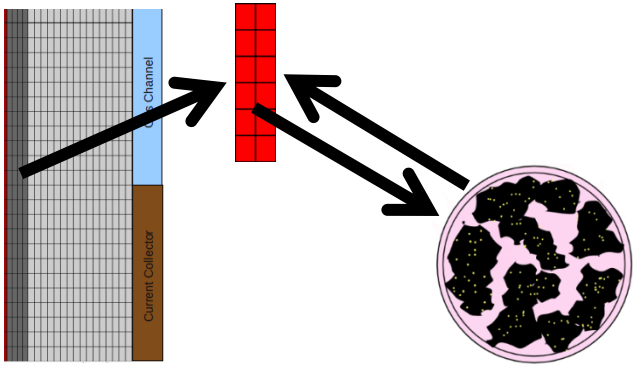






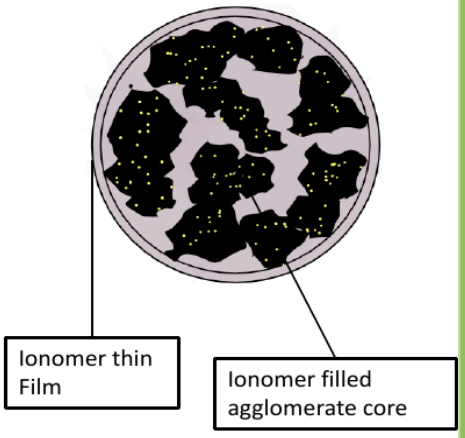
Effect of varied micro-structures in cathode electrode

Multi-scale coupling [3]



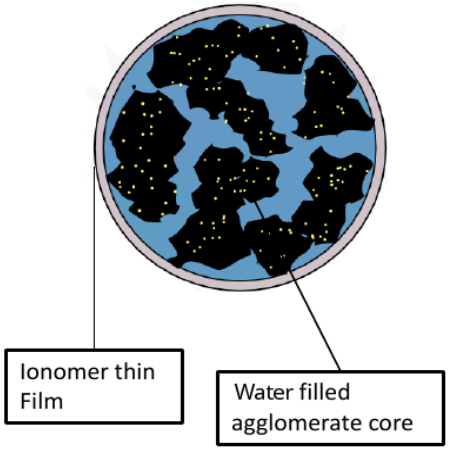
$$\nabla \cdot \vec{i} = \frac{1}{\frac{4}{3}\pi\left(1-\epsilon_V\right)\left(r_{agg}+\delta_{agg}\right)^3} \int_0^{r_{agg}} 4\pi r^2\, i(r,\vec{u})\, \mathrm{d}r.$$

Ionomer-filled [1]



$$\vec{\nabla} \cdot \left(\sigma_m^{eff} \vec{\nabla} \phi_m\right) = i$$
$$\vec{\nabla} \cdot \left(D_{O_2}^{eff} \vec{\nabla} c_{O_2}\right) = \frac{i}{4F}.$$

Water-filled [2]

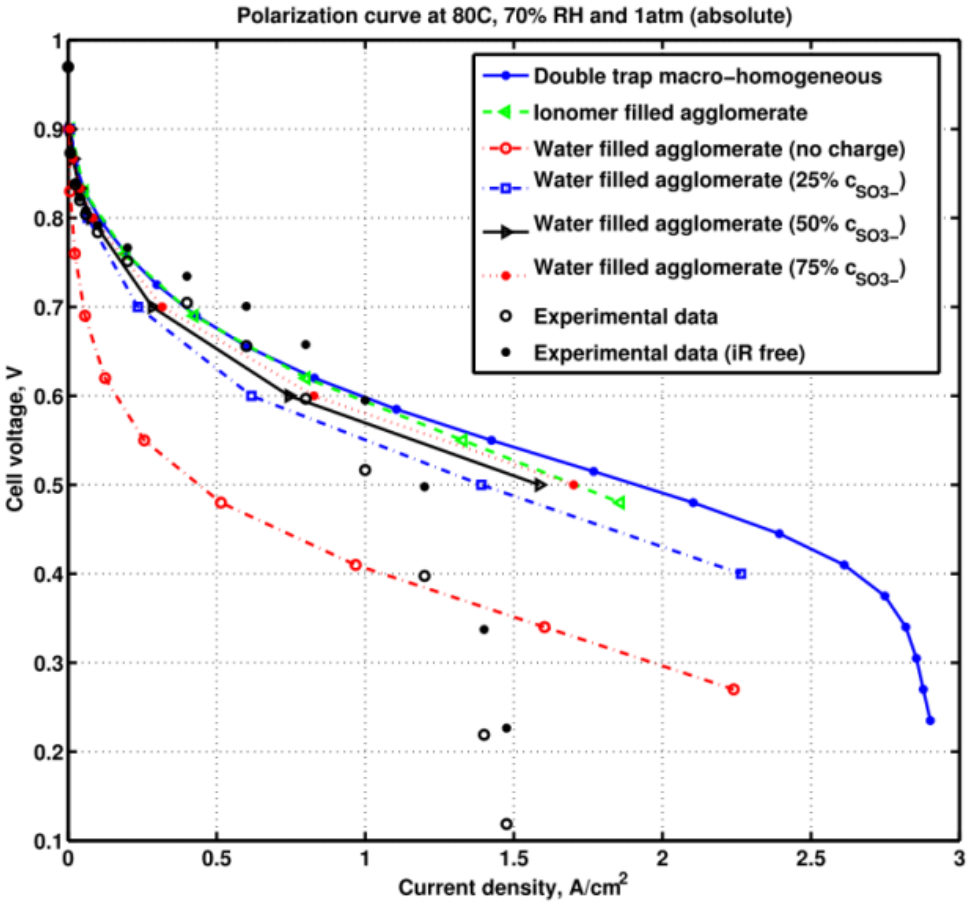


$$\vec{\nabla} \cdot [D_{H^+}^{eff}(\vec{\nabla} c_{H^+} + \frac{F}{RT} c_{H^+} \vec{\nabla} \phi_m)] = \frac{i}{F}$$
$$\vec{\nabla}^2 \phi_m = -\frac{F}{\varepsilon\varepsilon_0}(c_{H^+} - c_-)$$
$$\vec{\nabla} \cdot \left(D_{O_2}^{eff} \vec{\nabla} c_{O_2}\right) = \frac{i}{4F}.$$

1. Sun, W., Peppley, B. A., and Karan, K. Electrochimica Acta 50(16-17), 3347–3358, (2005).
2. Wang, Q., Eikerling, M., Song, D., and Liu, Z. Journal of Electroanalytical Chemistry, 573, 61–69 (2004).
3. Moore, M. et al., Journal of The Electrochemical Society 161(8), E3125–E3137 (2014).

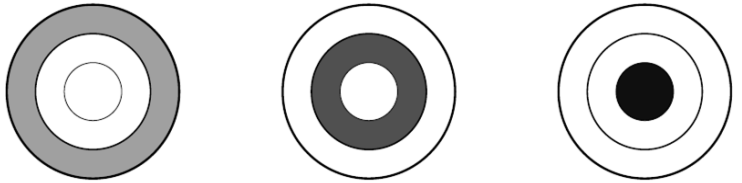
Effect of varied micro-structures in cathode electrode

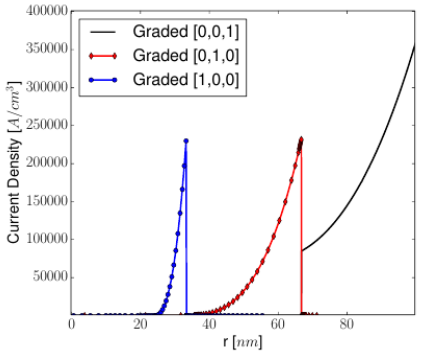
- Agglomerate parameters:
  - R_{agg} = 100 nm
  - δ_{agg} = 5.62 nm
  - 20% porosity
- Macro-homogeneous and agglomerate models show similar performance
- Water-filled model only appropriate if catalyst is negatively charged

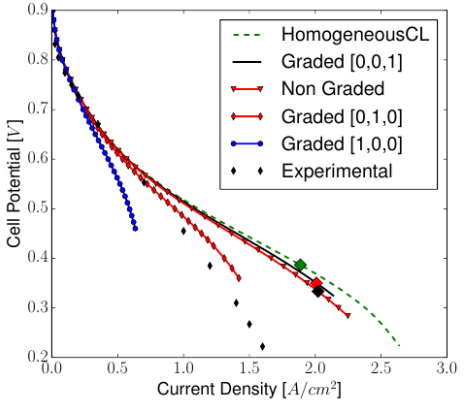


Effect of varied micro-structures in cathode electrode

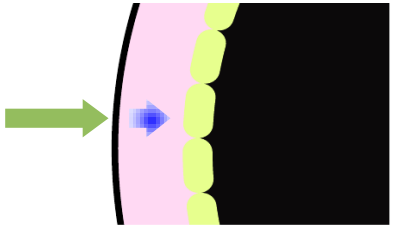
- Graded Platinum distribution:

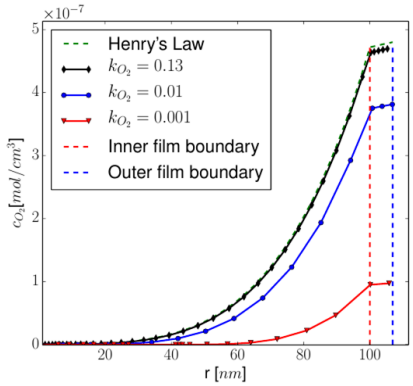


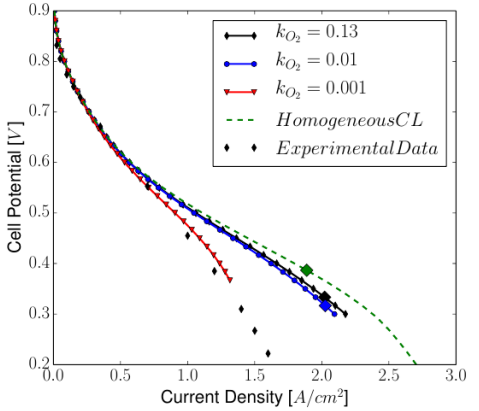




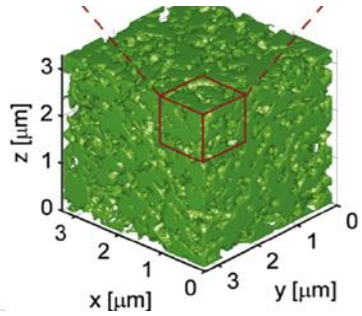
- Ionomer interfacial resistance:

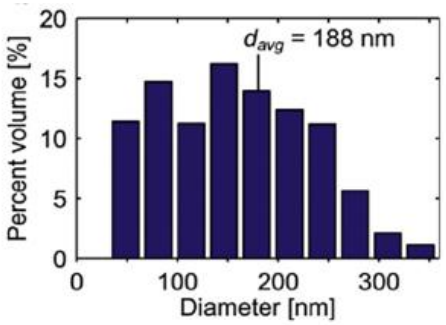


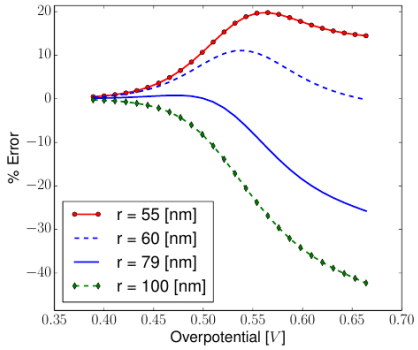


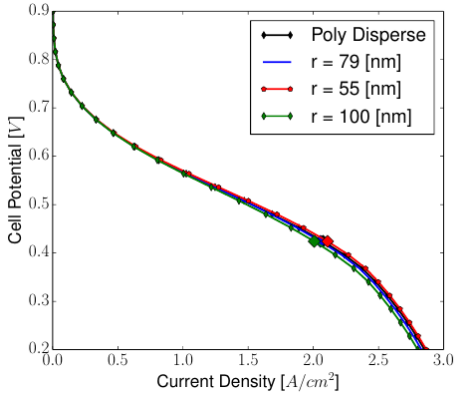


- Polydispersion of agglomerates:





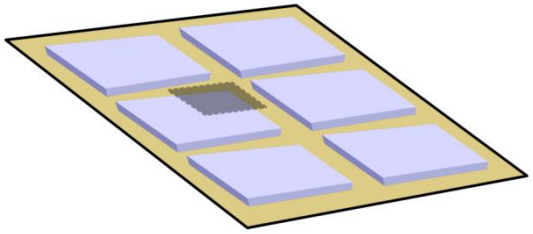


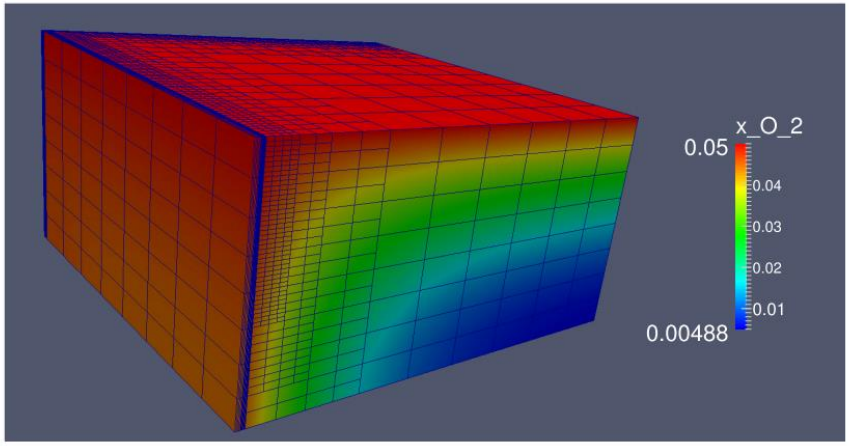


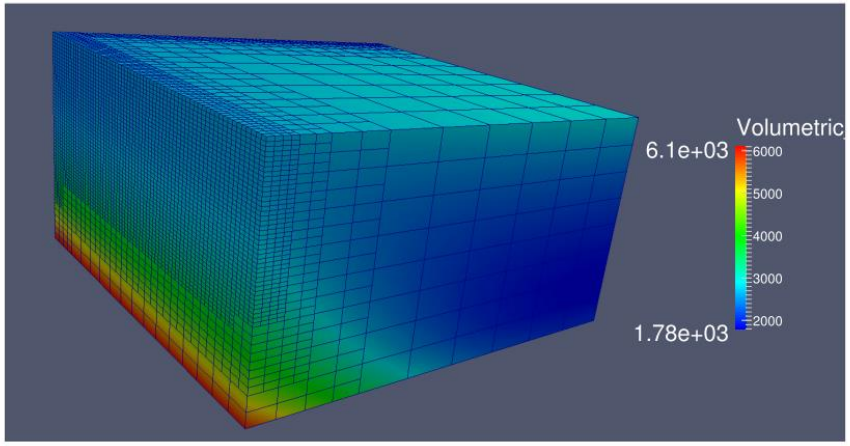
1.Epting W. K and Litster S. International Journal of Hydrogen Energy, 2012.

Patterned Electrode Analysis

- Inkjet printing used to pattern electrodes
- Effect of thickness and spacing between printed CL blocks analyzed in openFCST
- Reaction hot-spots observed







Conclusions

- An open-source numerical analysis framework has been developed for analyzing multi-dimensional fuel cells
  - Modular and easily extendable
  - Developed for (users and) developers
    - Release 0.2 (due November) will contain a GUI and will use CMake to improve installation issues in different environments
  - Developed in C++ using a Linux environment
  - Caution: Steep learning curve (but we are willing to help)
- The framework has been successfully applied to analyze:
  - Different electrochemical reaction models
  - Different micro-scale models
  - Perform three-dimensional catalyst layer simulations of patterned electrodes

Acknowledgement

Lab members:
Dr. Valentin Zingan, Shantanu Shukla, Lalit Pant, Pedro Mateo, Michael Moore, Madhur Bhaiya, Phil Wardlaw, Kailyn Domican, Derek Paxman, Mark Dumontier, Prafful Mangal, Alex Jarauta, Patrick Lohman, Simon Hoetzendorfer

Collaborators:
Dr. Minev, UofAlberta
Dr. Spiteri, USaskatchewan
Dr. Kanschat, UHeidelberg

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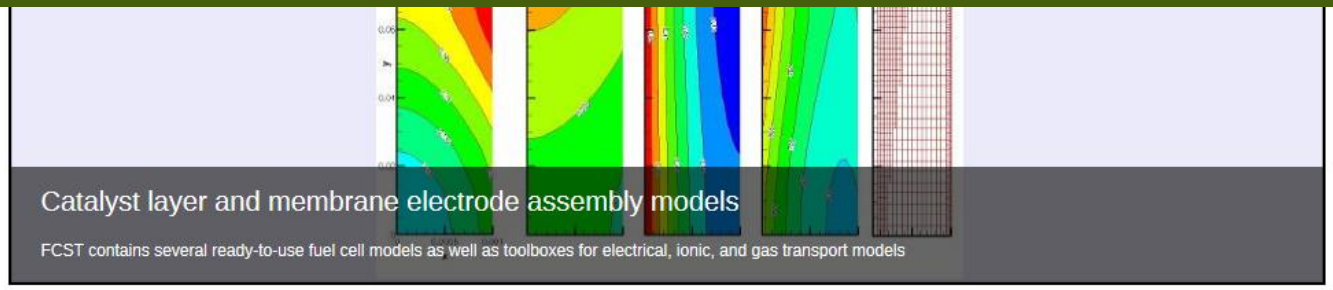
THANK YOU



OpenFCST: The Open-source Fuel Cell Simulation Toolbox

News

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