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Computational Modeling and Optimization of Proton Exchange Membrane Fuel Cells using deal.ii

Deal.ii Users Workshop

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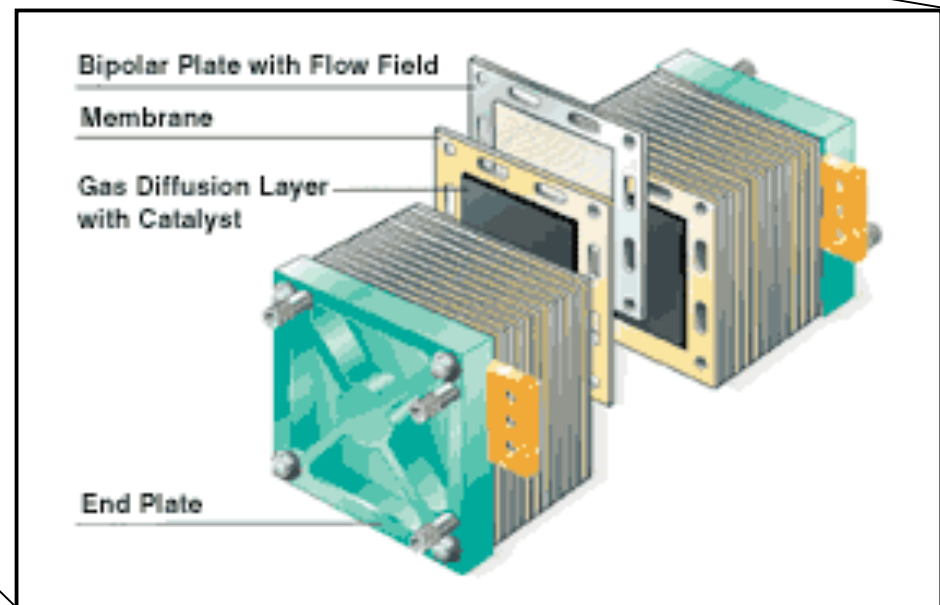
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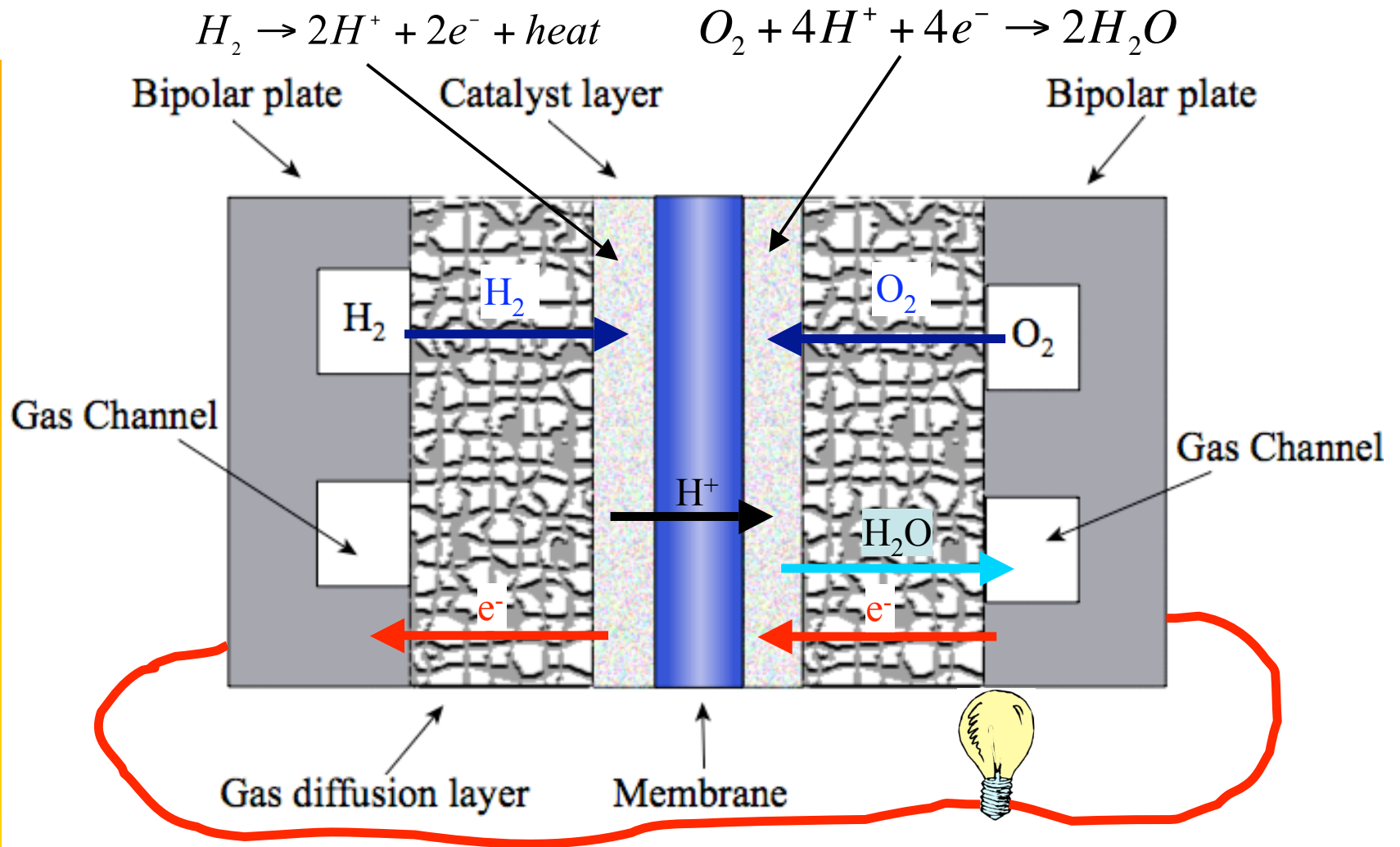
Introduction





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Introduction





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Introduction

- Fuel cells are governed by several coupled physical phenomena
- Fuel cell performance depends on a large number of coupled design parameters
- Numerical optimization allows changing of all design parameters simultaneously to obtain an optimal design



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Previous work

- Song et al., 2004
 - One-dimensional catalyst layer model
 - Gradient-based method with numerical sensitivities
- Gurujicic et al., 2004
 - Two- and three-dimensional fuel cell with a zero-thickness catalyst layer model
 - Gradient-based method with numerical sensitivities
- Mawardi et al., 2005
 - One-dimensional fuel cell model
 - Nelder-Mead simplex method combined with simulated annealing optimization



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Previous work

- Limited to a low accuracy fuel cell model due to the computational expense of solving high-fidelity models
- This limitation can be reduced by using
 - parallel machine architecture
 - gradient-based methods
 - efficient method to compute the gradients



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Objectives

- Development of an optimization framework for high-fidelity fuel cell models by using
 - accurate two-dimensional fuel cell models solved using deal.ii
 - gradient-based optimization algorithms coupled with analytical sensitivities obtained using deal.ii



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Methodology

- In order to develop a numerical fuel cell optimization framework it is necessary to develop
 - Accurate fuel cell model
 - A program using deal.ii to solve the fuel cell model
 - Appropriate objective function and constraints
 - Objective function and constraints analytical sensitivities
 - Optimization algorithm



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Fuel cell model

- Develop the set of partial differential equations (PDE) that governs the fuel cell

$$R(u, p) = 0$$

- Solve the governing equations using the deal.ii finite element library
- Adaptive mesh refinement
- Parallel solution of the equations



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Design problem

- Perform a parametric study and select
 - ✓ objective function
 - maximize current density
 - maximize power
 - ✓ constraints/requirements
 - limit maximum cell temperature
 - limit maximum amount of platinum
 - ✓ design variables
 - geometric variables
 - composition variables
 - operating variables



Analytical sensitivities

- Gradients of objective function and constraints, f , are given by

$$\frac{df(u, p)}{dp} = \frac{\partial f(u, p)}{\partial u} \frac{\partial u}{\partial p} + \frac{\partial f(u, p)}{\partial p}$$

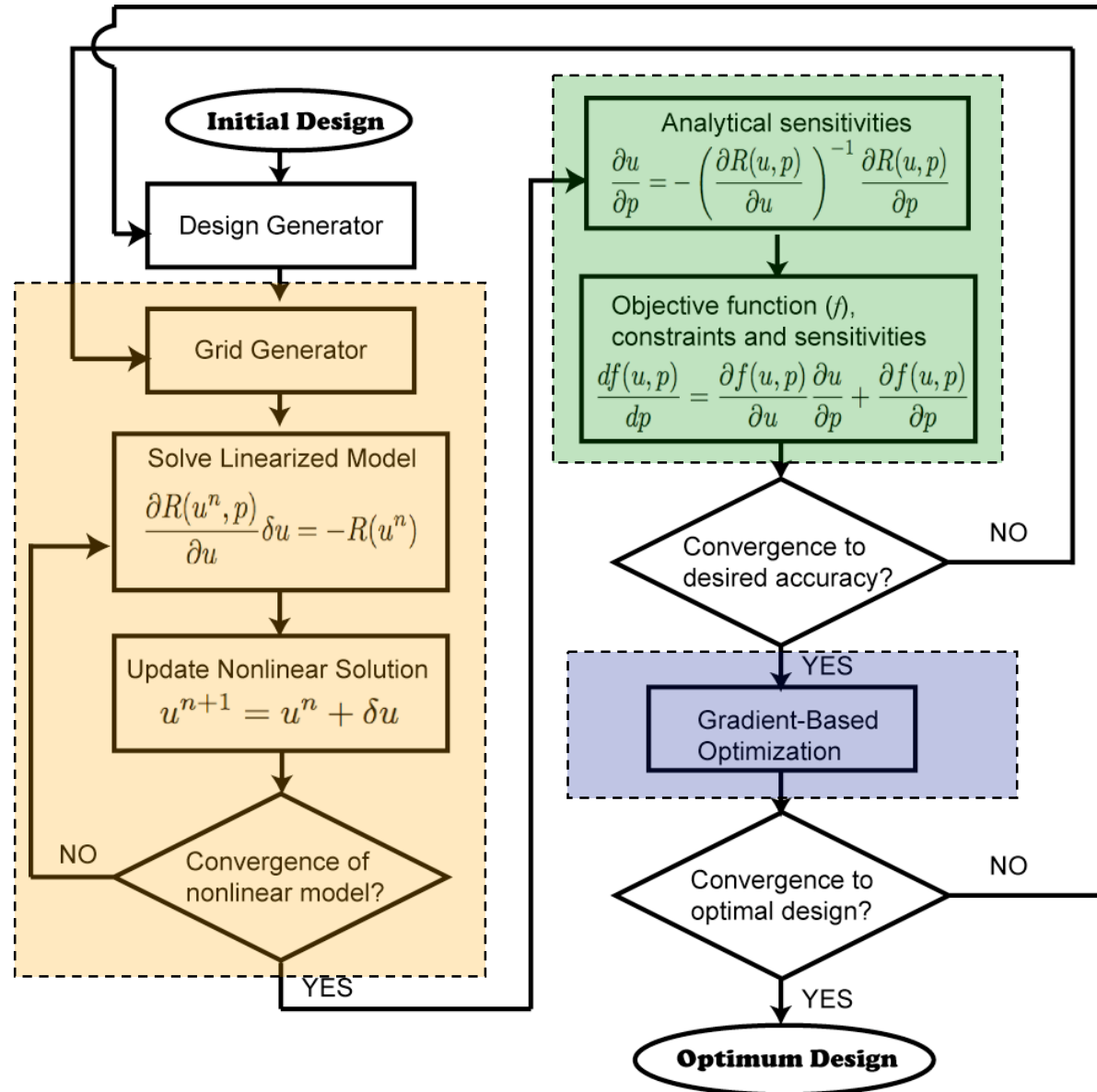
- Differentiate the fuel cell governing equations with respect to the design parameters

$$\frac{\partial R(u, p)}{\partial u} \frac{\partial u}{\partial p} = - \frac{\partial R(u, p)}{\partial p}$$



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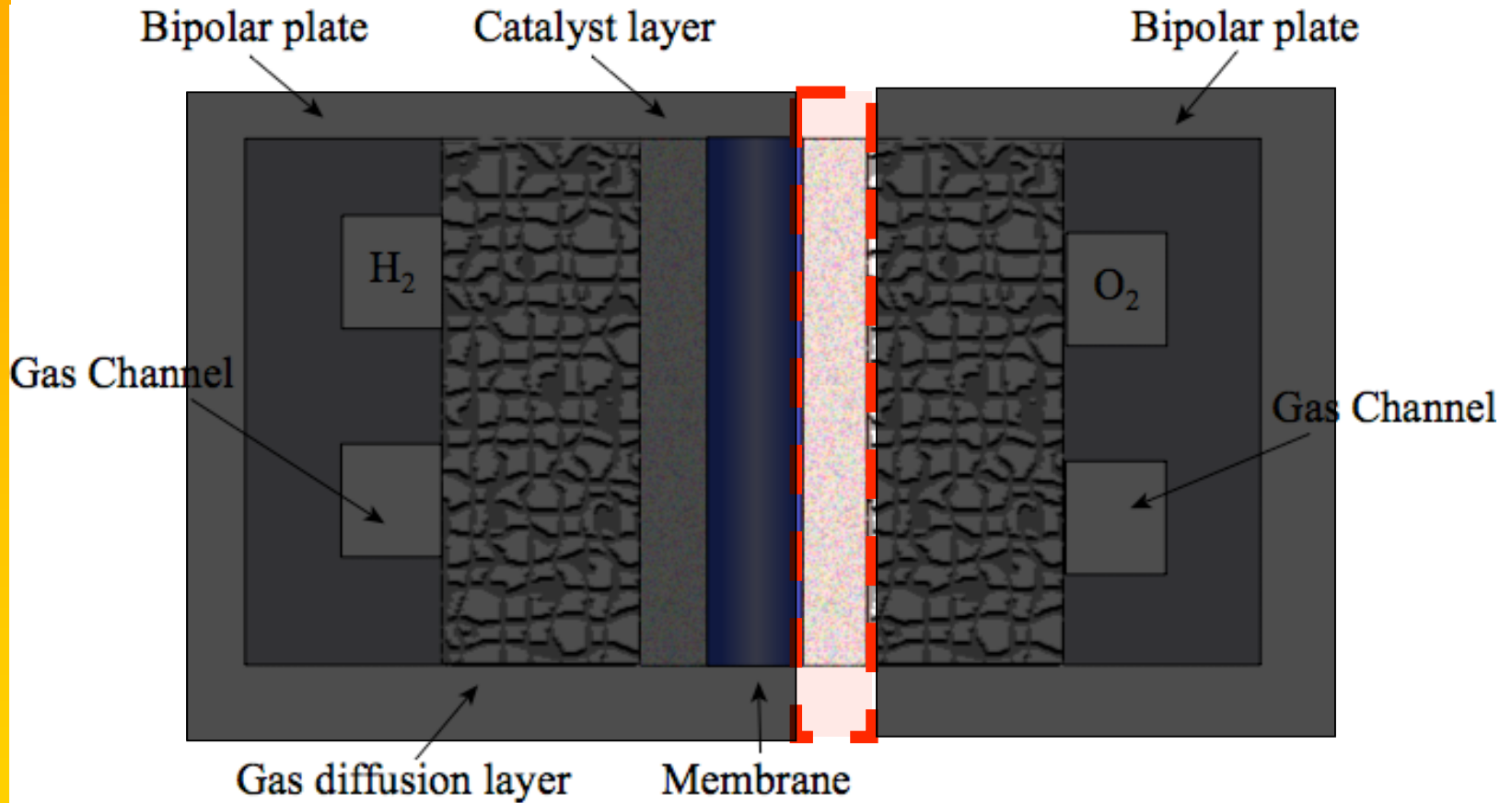
Optimization framework





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Catalyst layer optimization





Problem formulation

- One dimensional catalyst layer composition optimization
- Optimization problem is to

minimize $overpotential(\eta(i = i_0))$

w.r.t. ϵ_N, m_{Pt}

subject to: $0 \leq \epsilon_V \leq 1$

$0 \leq \epsilon_S \leq 1$

$0 \leq \epsilon_N \leq 1$



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1D catalyst layer model

$$\left. \begin{aligned} nFD_{O_2}^{eff} \frac{d^2 c_{O_2}}{dx^2} &= \frac{di}{dx} = f(c_{O_2}, \eta) \\ \left(\frac{-1}{\frac{1}{\sigma_N^{eff}} + \frac{1}{\sigma_S^{eff}}} \right) \frac{d^2 \eta}{dx^2} &= \frac{di}{dx} = f(c_{O_2}, \eta) \end{aligned} \right\}$$

where

$$f(c_{O_2}, \eta) = \frac{di}{dx} = i_0^{ref} \left(\frac{c_{O_2}}{c_{O_2}^{ref}} \right)^\gamma \exp \left(\frac{\alpha F}{RT} \eta \right)$$



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Boundary conditions

$$c_{O_2}(x = 0) = c^*$$

$$\left. \frac{\partial c_{O_2}}{\partial x} \right|_{x=L} = 0$$

$$\left. \frac{\partial \eta}{\partial x} \right|_{x=0} = -\frac{1}{\sigma_S^{eff}} i_{tot} \simeq 0$$

$$\eta(x = L) = dV \quad \text{or} \quad \left. \frac{\partial \eta}{\partial x} \right|_{x=L} = \frac{1}{\sigma_N^{eff}} i_{tot}$$



Finite element solution

- Use Newton method to solve the system. The linearized equations are

$$\frac{dR(u, \lambda)}{du} \delta u = -R(u, \lambda)$$

- The linearized problem is solved using
 - the Galerkin method
 - first order elements
 - Global refinement



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Optimization process

- The gradient of the overpotential and constraints is obtained by analytical differentiation of the governing equations
- The Modified Method of Feasible Directions is used to solve the optimization problem



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Problem initial parameters

- Current density:
 - $i_0 = 0.5 \text{ A/cm}^2$
- Initial Design:
 - Objective:
 - $\eta = -0.675514 \text{ V}$
 - Design variables:
 - $m_{\text{Pt}} = 3.332 \times 10^{-4} \text{ g cm}^{-2}$
 - $\varepsilon_{\text{N}} = 0.3$



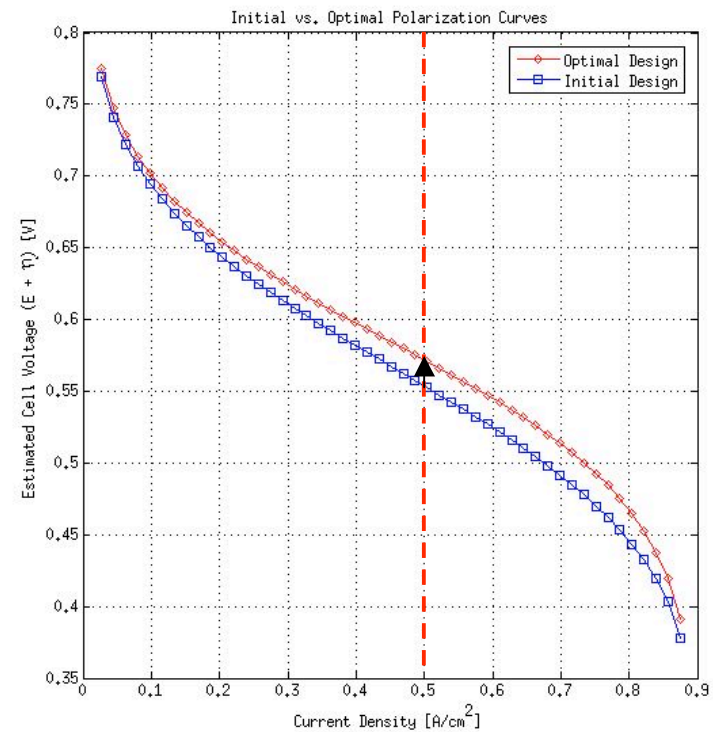
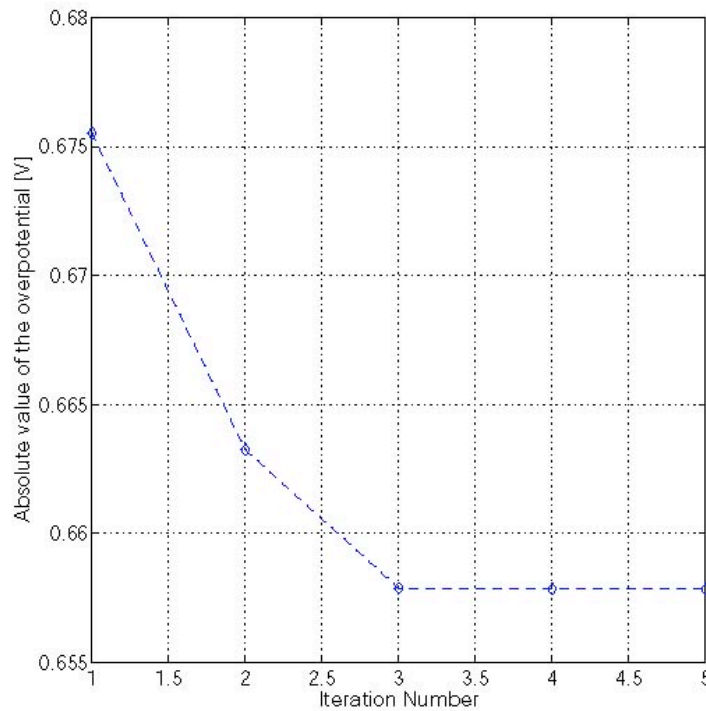
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Optimization results

- Optimal Design

✓ $\eta = -0.657852V$

✓ $m_{Pt} = 1.989 \times 10^{-4} \text{ g cm}^{-2}$, $\epsilon_N = 0.597806$

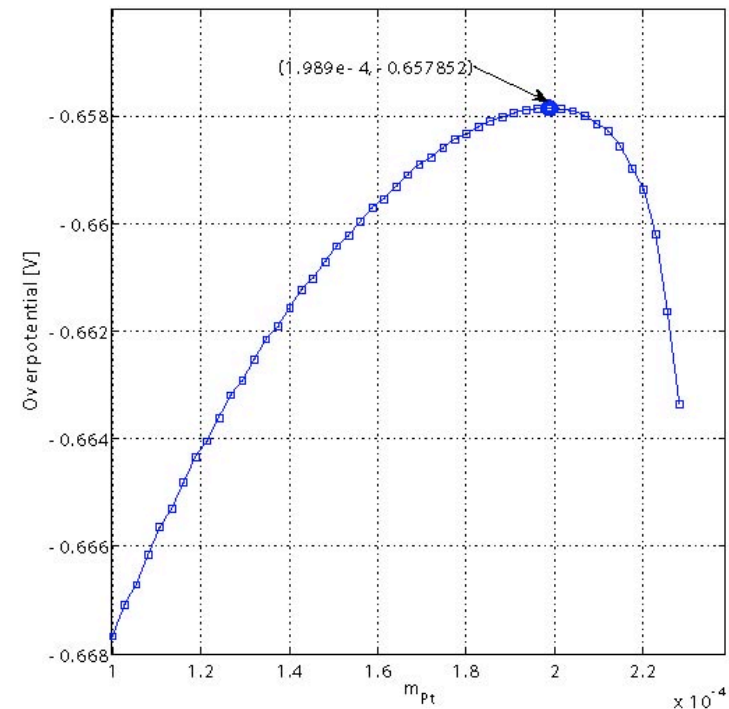
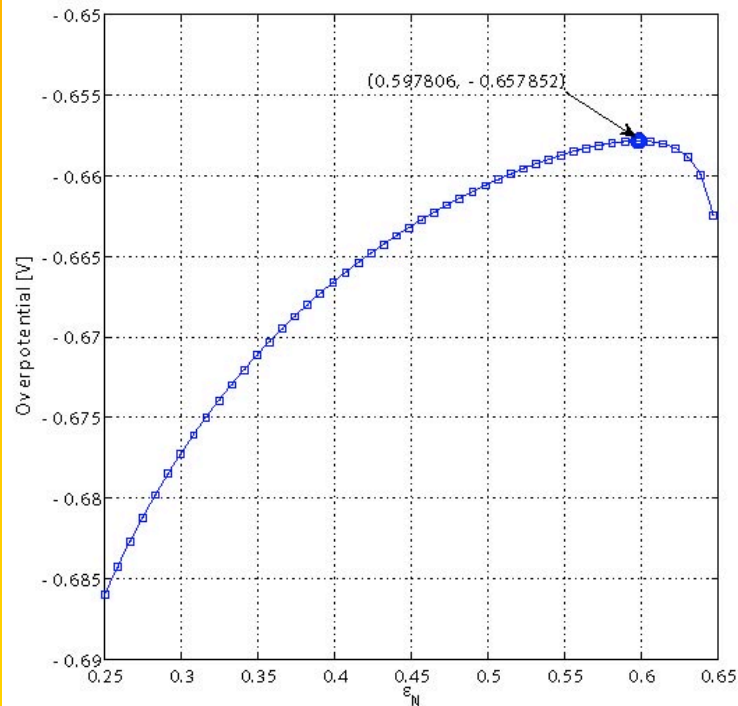




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Post-optimal analysis

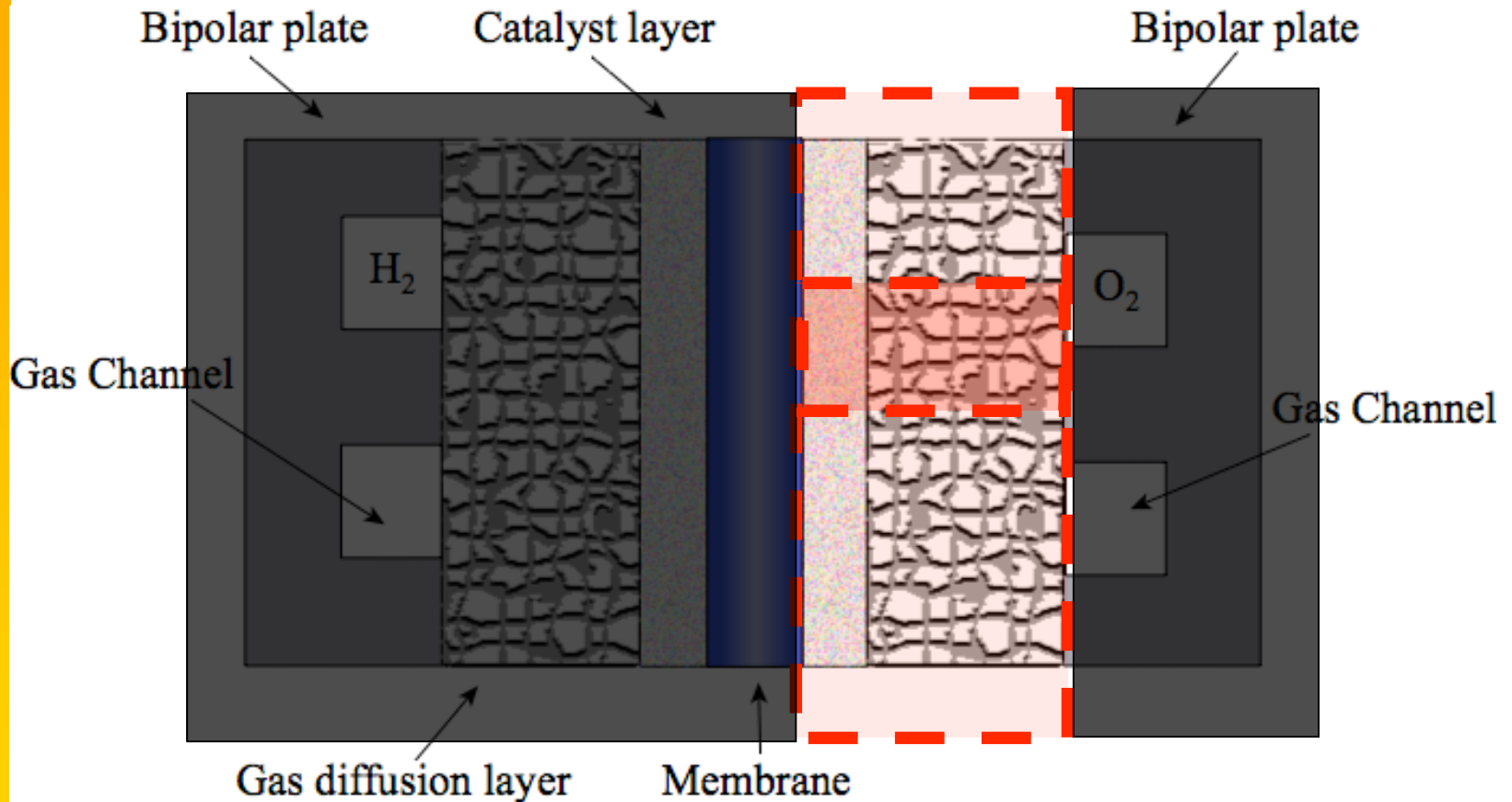
- Solution sensitivity to changes in design variables





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Two-dimensional cathode electrode optimization





Problem formulation

- Two dimensional electrode composition optimization
- Optimization problem is to

maximize $i(dV = V_0)$

w.r.t. $\epsilon_V^{GDL}, \epsilon_N^{CAT}, m_{Pt}, \%Pt$

subject to: $0 \leq \epsilon_V \leq 1$

$0 \leq \epsilon_S \leq 1$

$0 \leq \epsilon_N \leq 1$



Two-dimensional cathode electrode problem

$$\left. \begin{aligned} \nabla \cdot (cD_{O_2}^{eff} \nabla x_{O_2}) &= \frac{1}{4F} \nabla \cdot \vec{i} \\ \nabla \cdot (\sigma_m^{eff} \nabla \phi_m) &= \nabla \cdot \vec{i} \\ \nabla \cdot (\sigma_S^{eff} \nabla \phi_S) &= -\nabla \cdot \vec{i} \end{aligned} \right\}$$

where

$$\nabla \cdot \vec{i} = i_0^{ref} \left(\frac{cx_{O_2}}{c_{O_2}^{ref}} \right)^\gamma \exp \left(\frac{\alpha F}{RT} (\phi_m - \phi_S) \right)$$



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Boundary conditions

$$\vec{n} \cdot \nabla x_{O_2} = 0$$

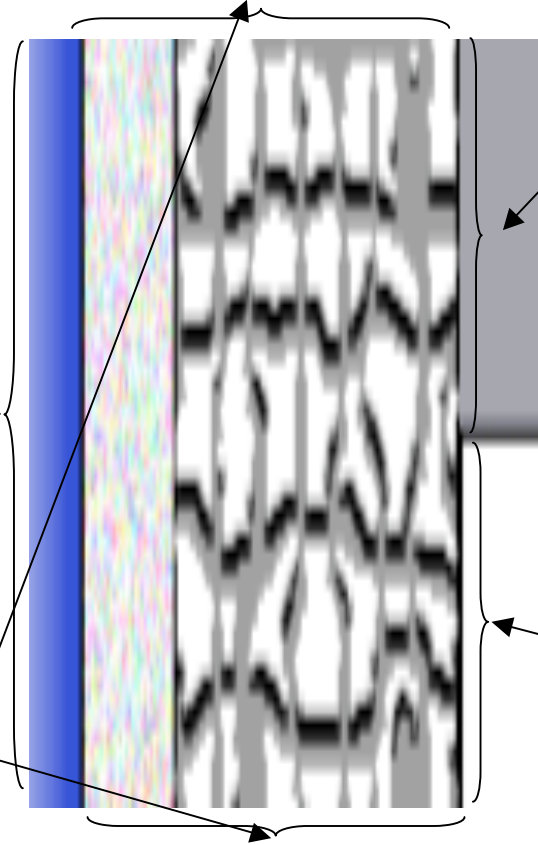
$$\vec{n} \cdot \nabla \phi_S = 0$$

$$\phi_m = \phi_0$$

$$\vec{n} \cdot \nabla x_{O_2} = 0$$

$$\vec{n} \cdot \nabla \phi_S = 0$$

$$\vec{n} \cdot \nabla \phi_m = 0$$



$$\vec{n} \cdot \nabla x_{O_2} = 0$$

$$\phi_S = 0$$

$$\vec{n} \cdot \nabla \phi_m = 0$$

$$x_{O_2} = x_{O_2}^0$$

$$\vec{n} \cdot \nabla \phi_S = 0$$

$$\vec{n} \cdot \nabla \phi_m = 0$$



Finite element solution

- Use Newton method to solve the system of equations. The linearized equations are

$$\frac{dR(u, \lambda)}{du} \delta u = -R(u, \lambda)$$

- The linearized problem is solved using
 - the Galerkin method
 - first order elements
 - adaptive grid refinement



Current density

- The current density is obtained in the post-analysis using either

$$i = \frac{1}{H} \int_0^H \int_0^L RR dx dy =$$
$$= \frac{1}{H} \int_0^H \int_0^L i_0^{ref} \left(\frac{cx_{O_2}}{c_{O_2}^{ref}} \right)^\gamma \exp \left(\frac{\alpha F}{RT} (\phi_m - \phi_S) \right) dx dy$$

or

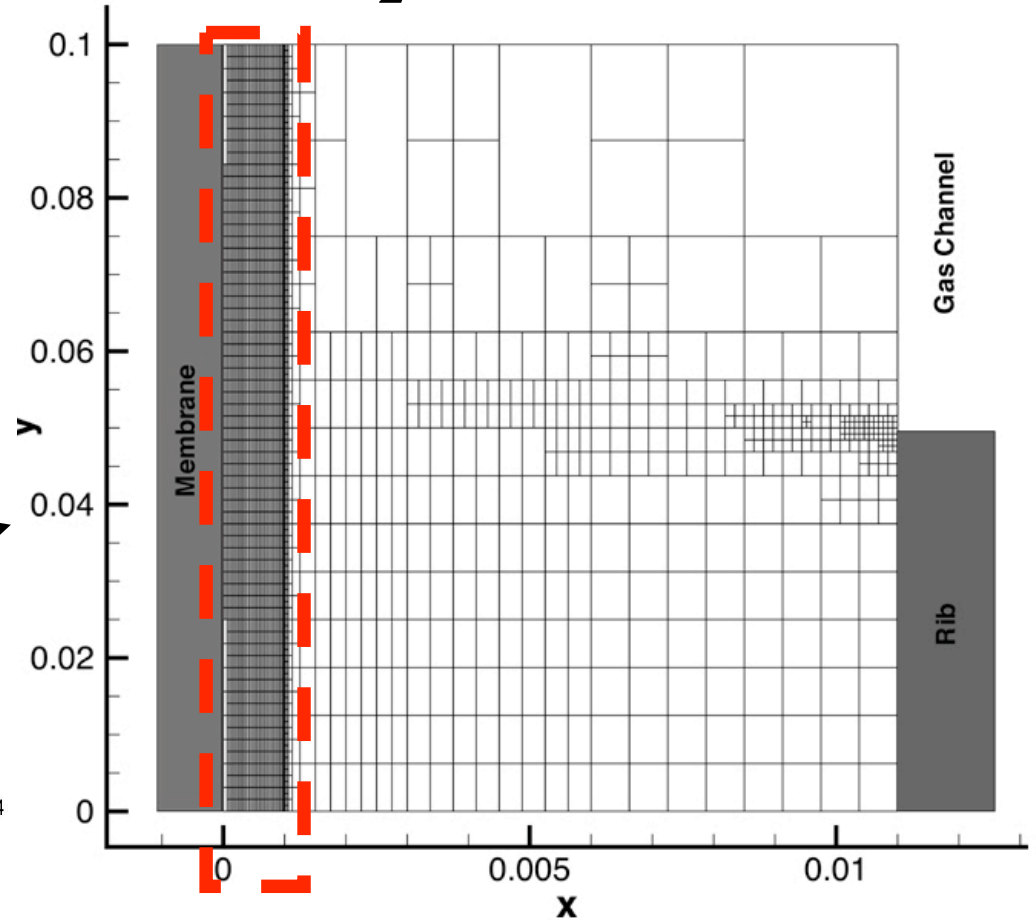
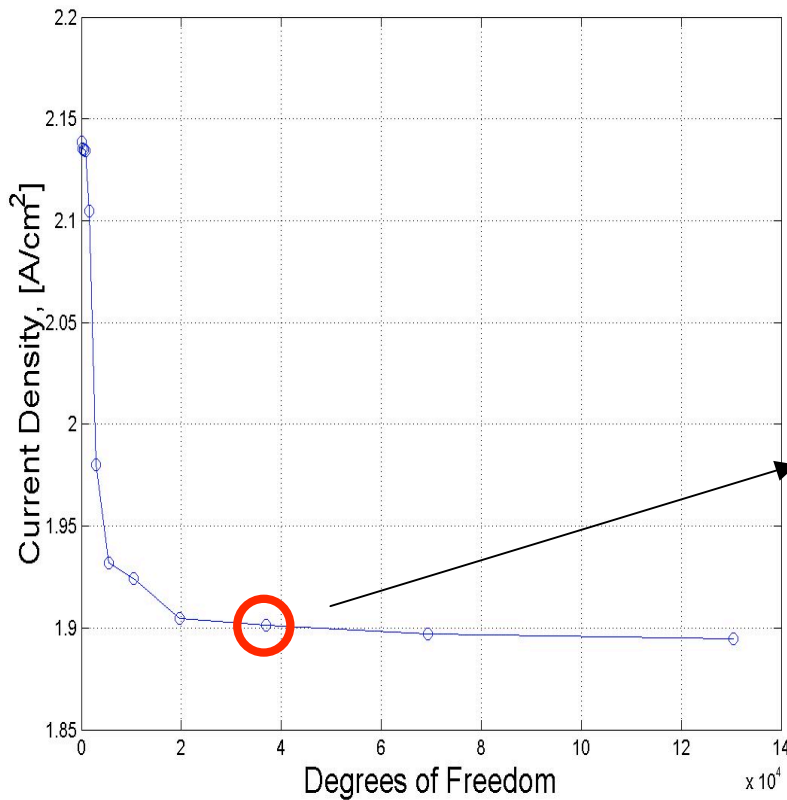
~~$$i = \frac{1}{H} \int_0^H \sigma_m \nabla \phi_m dy$$~~



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Adaptive grid refinement

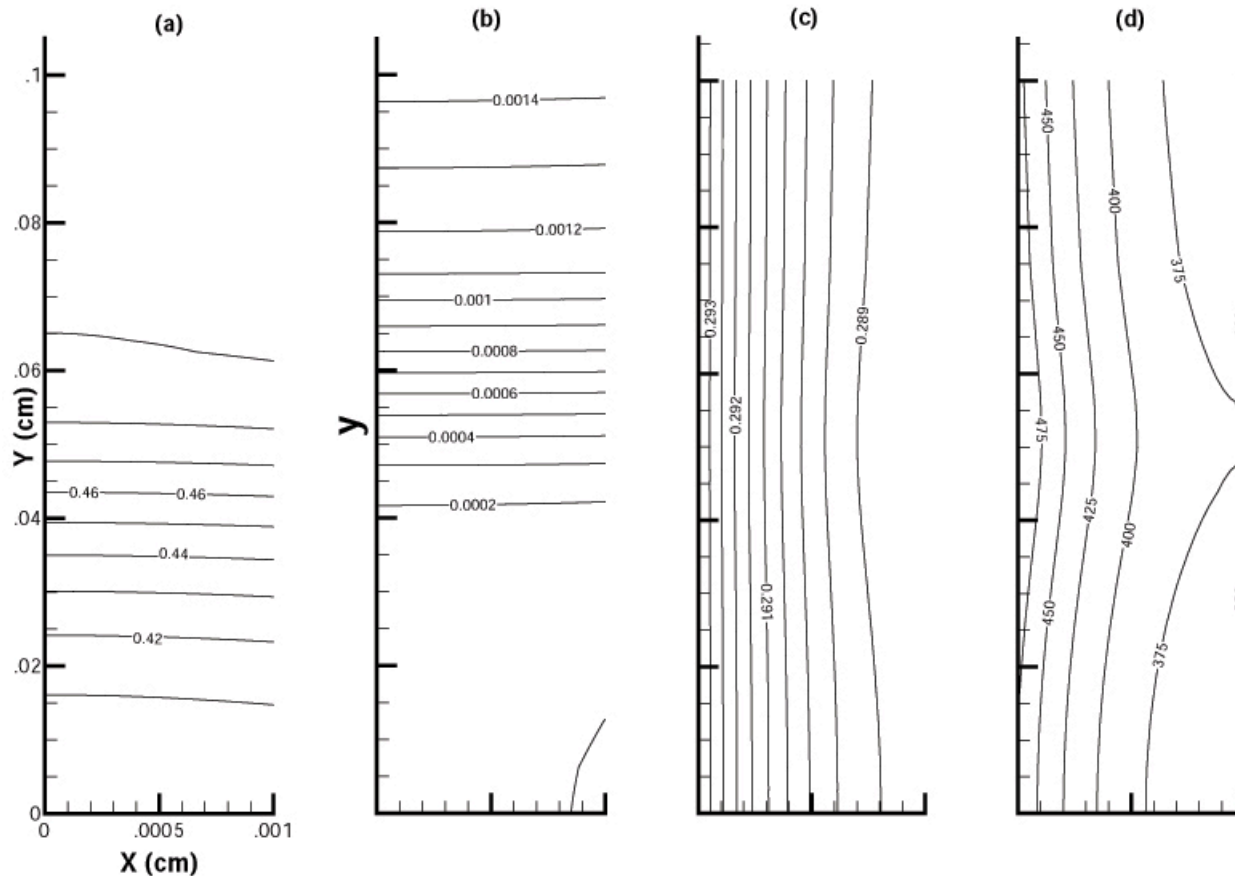
- Kelly error estimator for c_{o_2} and ϕ_S





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Catalyst layer solution



Contour lines at the catalyst layer for $i=0.4\text{A/cm}^2$ and $\sigma_s = 0.53\text{ S/cm}$ of
(a) oxygen molar fraction [-], (b) potential in the solid phase [V], (c)
potential in the electrolyte [V] and (d) reaction rate [A/cm^3]



Optimization solution

- Initial Design:
 - Objective:
 - $i = 0.491367 \text{ A/cm}^2$ for $dV = 0.25 \text{ V}$
 - Design variables:
 - GDL : $\varepsilon_V = 0.5$
 - CL: $m_{Pt} = 3.332 \times 10^{-4} \text{ g cm}^{-2}$
 - CL: $\varepsilon_N = 0.3$
 - CL: $\%Pt = 0.2$
 - Grid with a maximum of 500 dof => preliminary results!



Optimization solution

- Final Design:
 - Objective:
 - $i = 1.01408 \text{ A/cm}^2$ for $dV = 0.25 \text{ V}$
 - Design variables:
 - GDL : $\varepsilon_V = 0.620494 \Rightarrow \sim 25\%$ increase
 - CL: $m_{Pt} = 10.3464 \times 10^{-4} \text{ g cm}^{-2} \Rightarrow \sim 200\%$ increase
 - CL: $\varepsilon_N = 0.424708 \Rightarrow \sim 30\%$ increase
 - CL: $\%Pt = 0.463985 \Rightarrow \sim 60\%$ increase

The current density has doubled!!!



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Summary

- Deal.ii was successfully used
 - to solve one and two-dimensional fuel cell models involving highly nonlinear source terms
 - to obtain the analytical sensitivities of the unknowns of the analysis problem and the objective function of the optimization problem
 - to perform fuel cell optimization in conjunction with a commercial optimization software



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Thank You

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