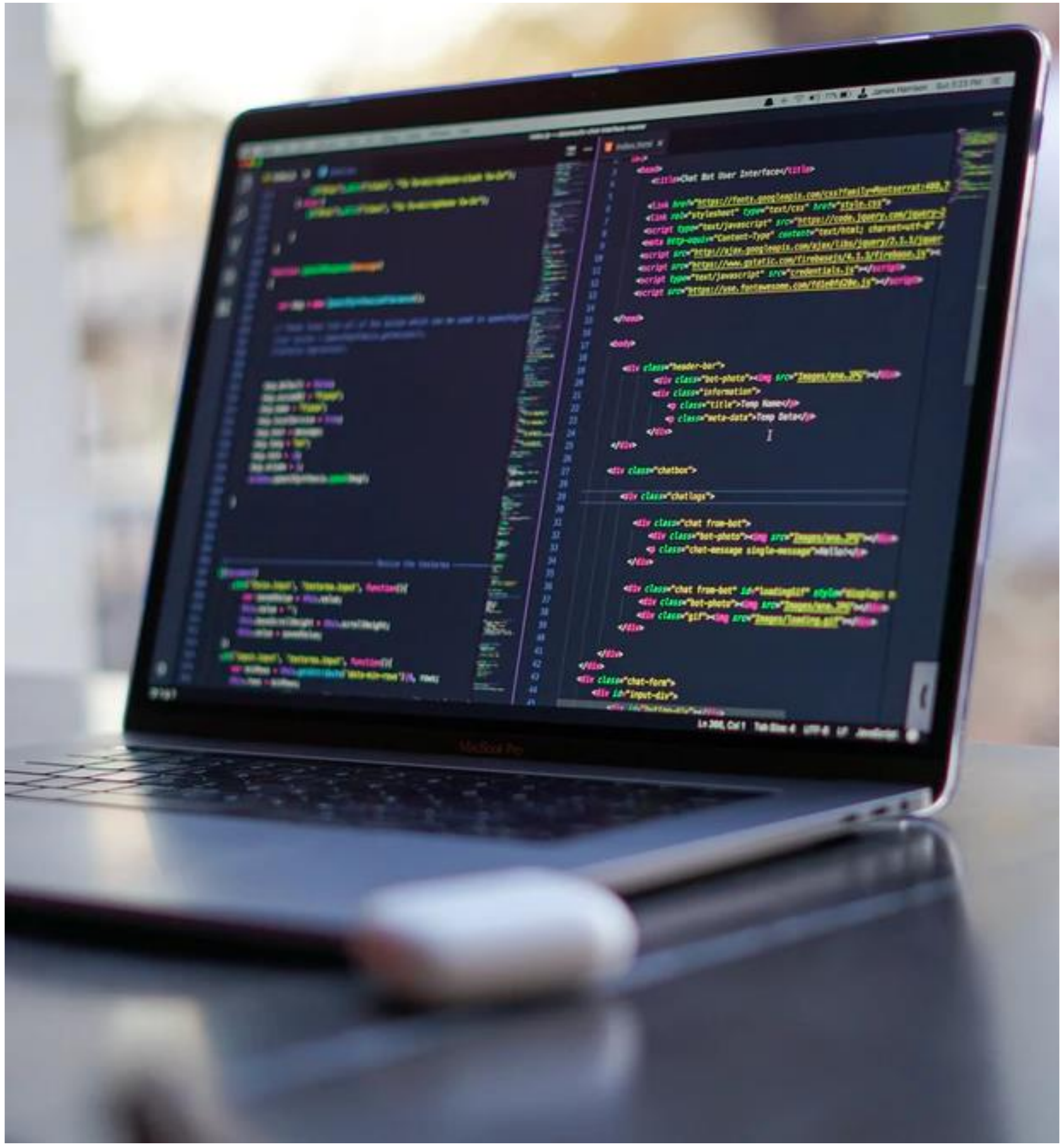


University of Alabama | Department of Chemical and Biological Engineering

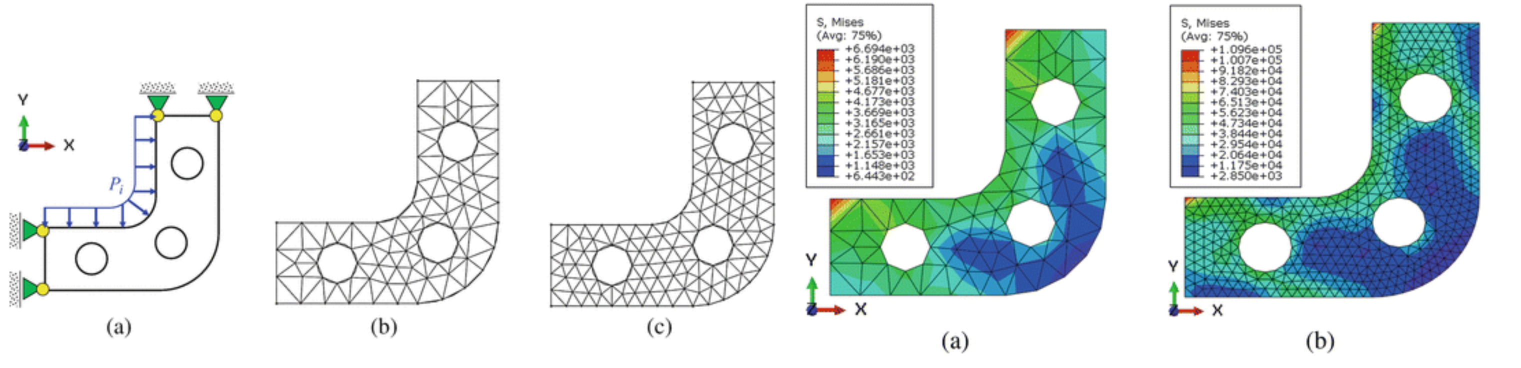
Finite Element Methods for Modern Engineering Applications

Shuvodeep De

Chemical and Biological Engineering, University of Alabama

Background

- High-speed computation has revolutionized simulation tools in science and engineering[1-24]
- Finite Element Methods have become popular for solving differential equations describing complex natural phenomena
- Algorithms are used on large systems to discretize them into a finite number of smaller parts called elements
- A broad class of functions is used to approximate a solution for each element
- **Finite Element Analysis finds application in several branches of Engineering including Aerospace, Automobile, Chemical and Biological**



Stress determination by Finite Element Method

Source: https://link.springer.com/chapter/10.1007/978-3-319-67125-3_6/

Aerospace

- **Bio-inspired Design of Aircraft Wing (with curvilinear Spars and Ribs)**
  - Computational framework to automate geometry and mesh generation, analysis, optimization and postprocessing

Automobile

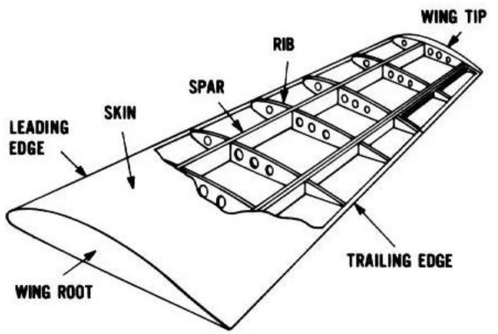
- **Lightweight Chassis Design for Hybrid Super Trucks**
  - Finite element model of truck chassis and validation
  - Computation framework to automate modelling, optimization and postprocessing

Chemical

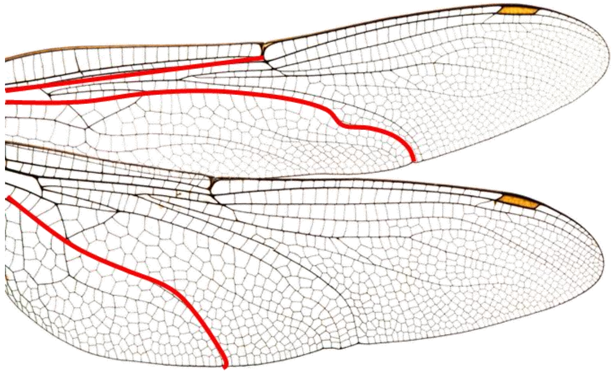
- **Manufacturing Defect-free Interconnects of Integrated Circuits by Electrodeposition of Metals**
  - Finite element model to predict copper growth
  - Chemical kinetic parameters estimated by mathematical model and used as input

Bio-inspired design of Aircraft Wings

Motivation

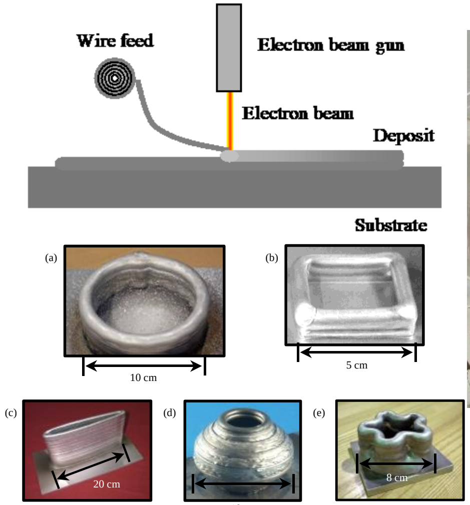


Wing Internal Structure#



Dragonfly wing *

Sailboat $



EBF3 in 0-g experiment (Courtesy: *Taminger*)

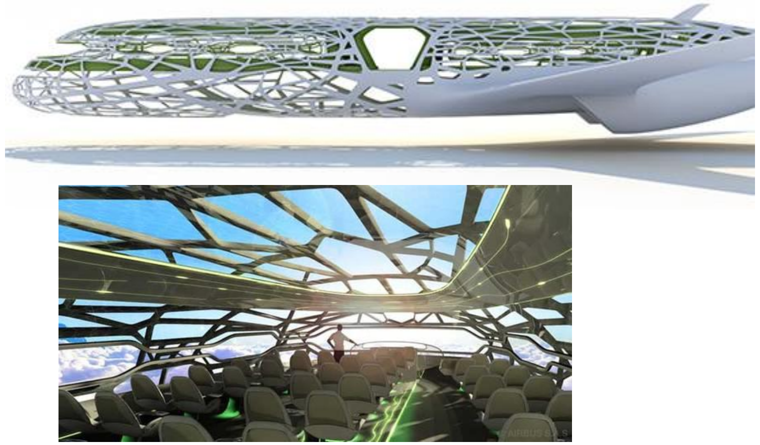
Electronic beam free form fabrication (EBF3) for 3D printing, *Taminger and Hafley 2003*

- Biologically inspired arbitrarily shaped stiffeners for structural design
- Stringers (veins) along wings of creatures are not always straight, which are mixed by curved and straight stringers (veins)
- Development of additive manufacturing technology for 3D printings of metal structures

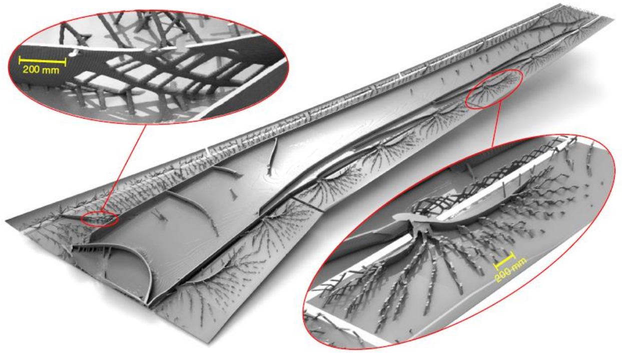
https://pdxscholar.library.pdx.edu/honorstheses/538/
*http://www.publicdomainpictures.net/viewimage.php?image=25114&picture=&jazyk=CN
$http://compositesmanufacturingmagazine.com/2018/03/lehvoss-sponsors-team-developing-worlds-first-3-d-printed-boat/

Motivation

- **Bio-Inspired Futuristic Aircraft Design**
  - Attempt to develop new type of aircraft using shape, size and topology optimization
  - Bionic structural design that mimics the bone structure of birds
  - Bone is light and strong; its porous interior carries tension only where necessary, leaving space elsewhere
  - Reduces aircraft's weight and fuel burn
- **Objective:**
  - A step forward in the direction to design futuristic aircraft structures
  - Implement the use of curvilinear/ arbitrary stiffeners for achieving better designs of structures



Bio-Inspired Futuristic Aircraft*



Wing design by Topology Optimization

Source: http://www.nature.com/doifinder/10.1038/nature23911/

**Image credit: AIRBUS*

Wing Optimization Problem

Static Aeroelasticity

- Stress < Yield Strength
- Displacement Constraints
  - Maximum Displacement < 12.5% Span
- Twist Angle Constraints
  - Twist Angle at Wing Tip < 6 Degrees

Bucking Aeroelasticity

- Buckling Factor of each panel >1
- Buckling Factor of entire wing >1

Flutter Analysis

- Find Critical Flutter Dynamic Pressure
- Flutter Constraint:
  - Flutter Dynamic Pressure >1.75 × 1.2 psi

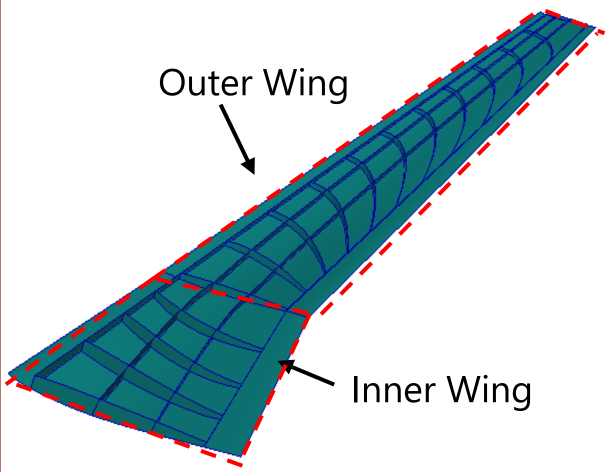
Flutter Video:
https://www.youtube.com/watch?v=egDWh7jnNic

Objective Function

$$\boldsymbol{f} = \frac{\boldsymbol{W}}{\boldsymbol{W_0}} + \sqrt{\frac{\boldsymbol{V_0}}{\boldsymbol{V_f}}}$$

W_0=10 lbs
V_0=158.11 knots

W: Weight (lbs)
V_f: Flutter speed (knots)
W_0: Effective weight (lbs)
V_0: Effective Flutter velocity (knots)

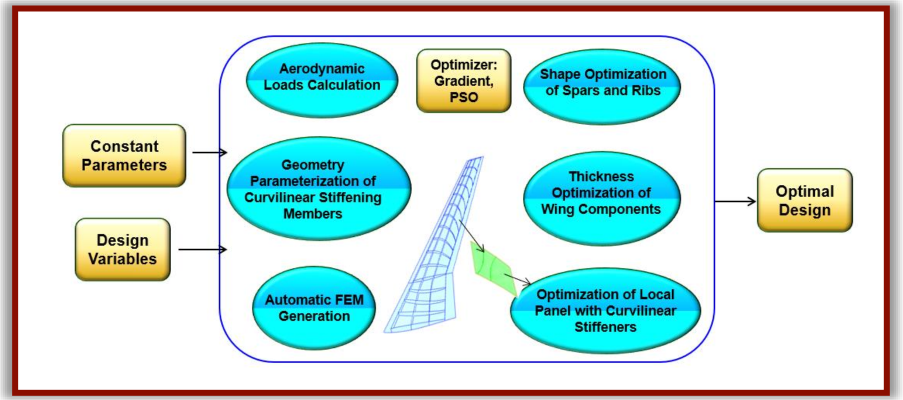


NASA Common Research Model

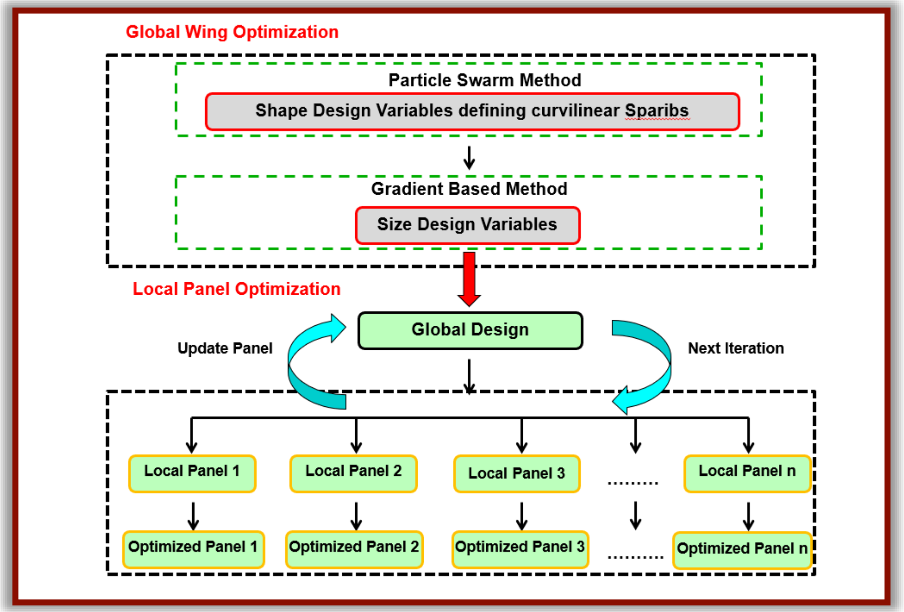
- Cruise Speed: Mach 0.85 at 35000 ft
- Angle of Attack: -2, 0, 2, 4, 6 degrees
- Total Span 192.7 ft
- Aspect Ratio AR = 9.0
- Quarter-Chord Sweep 35 Degrees

EBF3WingOpt Software (VT in-house code)

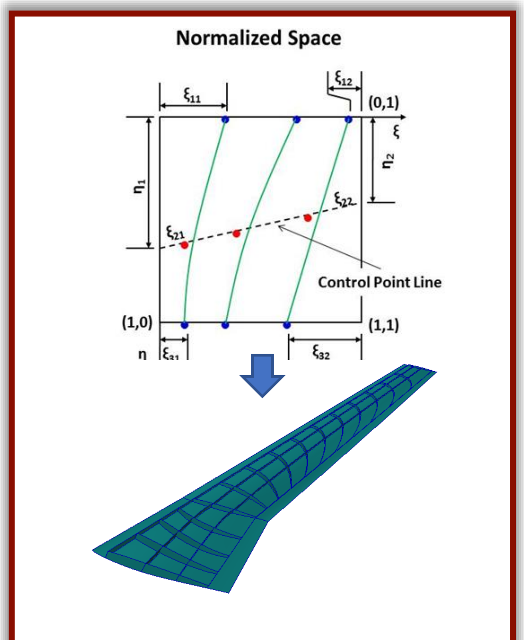
Multi-Disciplinary Analysis(MDA)



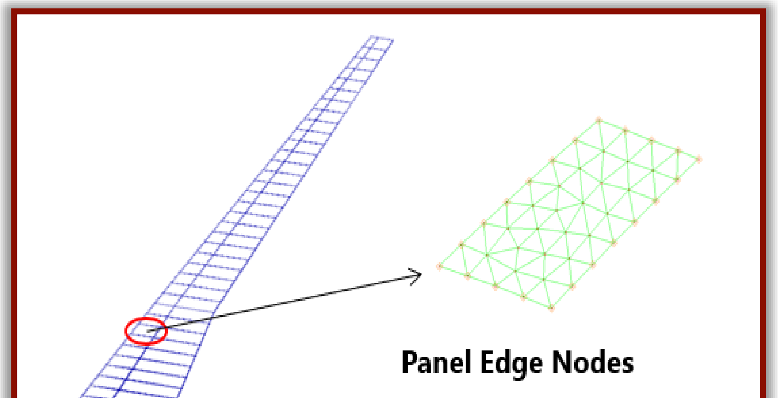
Multi-level Optimization(MDO)



- Automatic Geometry Parameterization and Mesh Generation of Aircraft Wing with curvilinear spars and ribs (***SpaRibs***)
- Integration of Static Aeroelastic Analysis, Flutter Analysis and Buckling Analysis
- ***Global Wing Optimization:*** Shape and Sizing optimization for the Wing Skins, Spars and Ribs
- ***Local Panel Optimization:*** Sizing optimization implemented for each panel subjected to the stress and buckling constraints



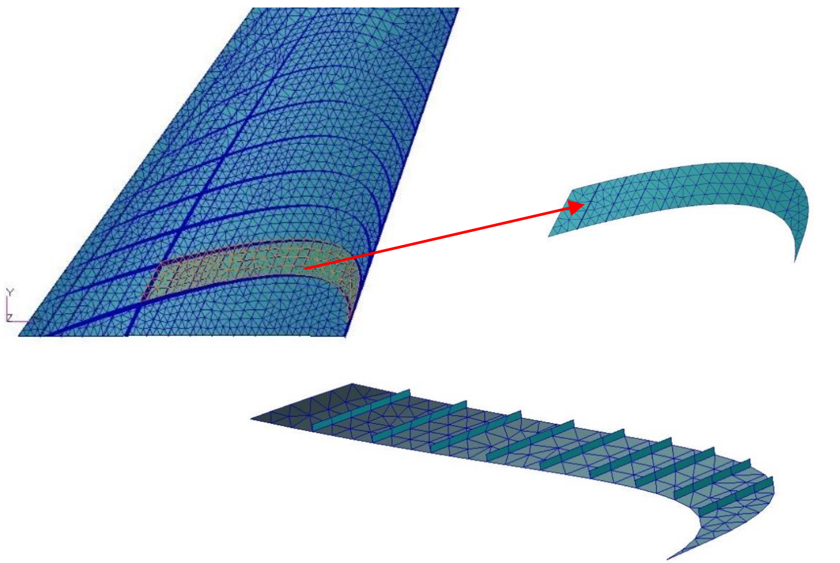
Geometry Generation



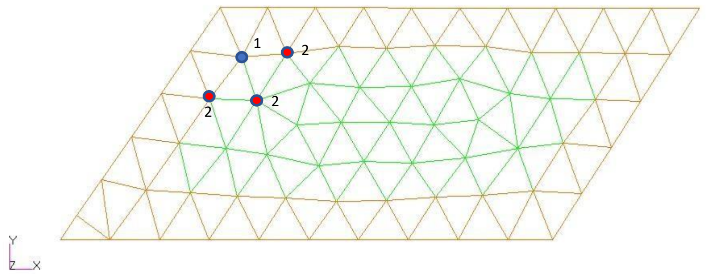
Local Panel Generation

Mesh Decomposition Algorithm

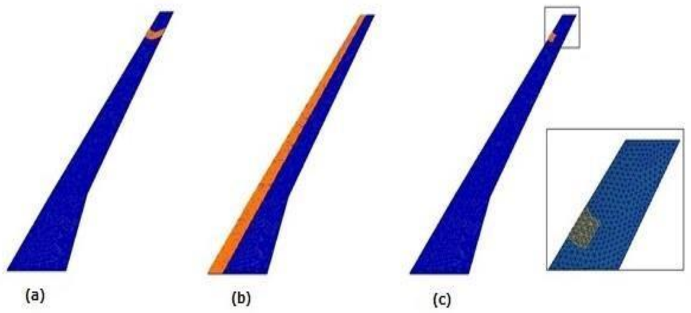
- Curvilinear Spars and Ribs (***SpaRibs***) parameterized using B-Splines
- Partial-depth Stiffener used to reinforce the panel
- Stiffener profile independent of panel shape
- Finite element model of each local panel is determined from the global model using in-house code



Isometric View of Local Panels with Stiffeners



Boundary Elements (red) and one Interior Node (Black) required to find all Elements of a Panel



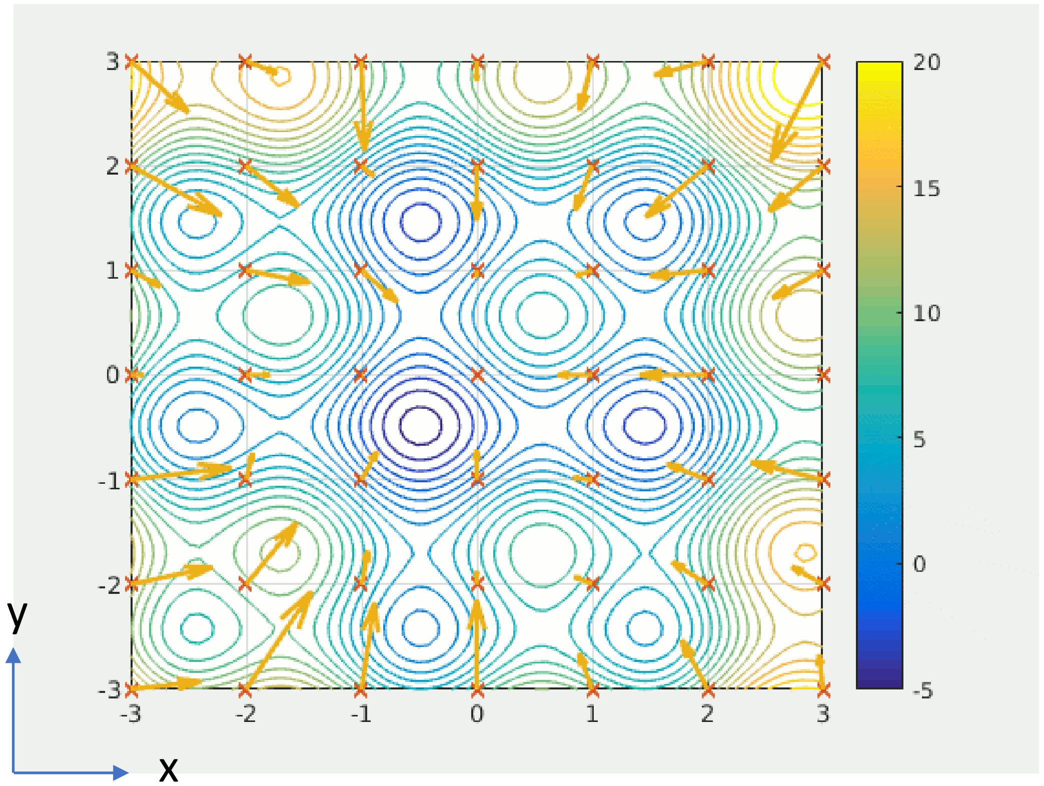
Skin Section between two Ribs (b) Skin Section between two Spars (c) Local Panel bounded by SpaRibs (Enlarged View provided in the Adjacent Box)

Particle Swarm Optimization

- Metaheuristic algorithm not requiring gradient information
- Algorithm inspired by behavior of flock of birds
- Set of random ***particles*** **(Designs)** defined over full domain
- ***Objective function* is *evaluated*** for every particle
- ***Design variable*** of the particles are ***improved based on*** a particle's ***own best value*** and the ***global best value*** in the entire swarm
- Discovery of ***improved positions*** become a ***guide*** for movements of the swarm
- After each iteration, new values are found using:
  - $v_{k+1}^{i} = w\, v_{k}^{i} + \frac{r_1\left(p^{i} - x_{k}^{i}\right)}{\Delta t} + \frac{r_2\left(p_{k}^{g} - x_{k}^{i}\right)}{\Delta t}$
  - $x_{k+1}^{i} = x_{k}^{i} + v_{k+1}^{i} \Delta t$

Where,

- w, weighting parameter, balance between local and global search
- r_1 and r_2 are random numbers varying from 0 to 1
- Δt, time step is generally taken unity
- p^{i} and p_{k}^{g} are particle's own best position and best swarm position

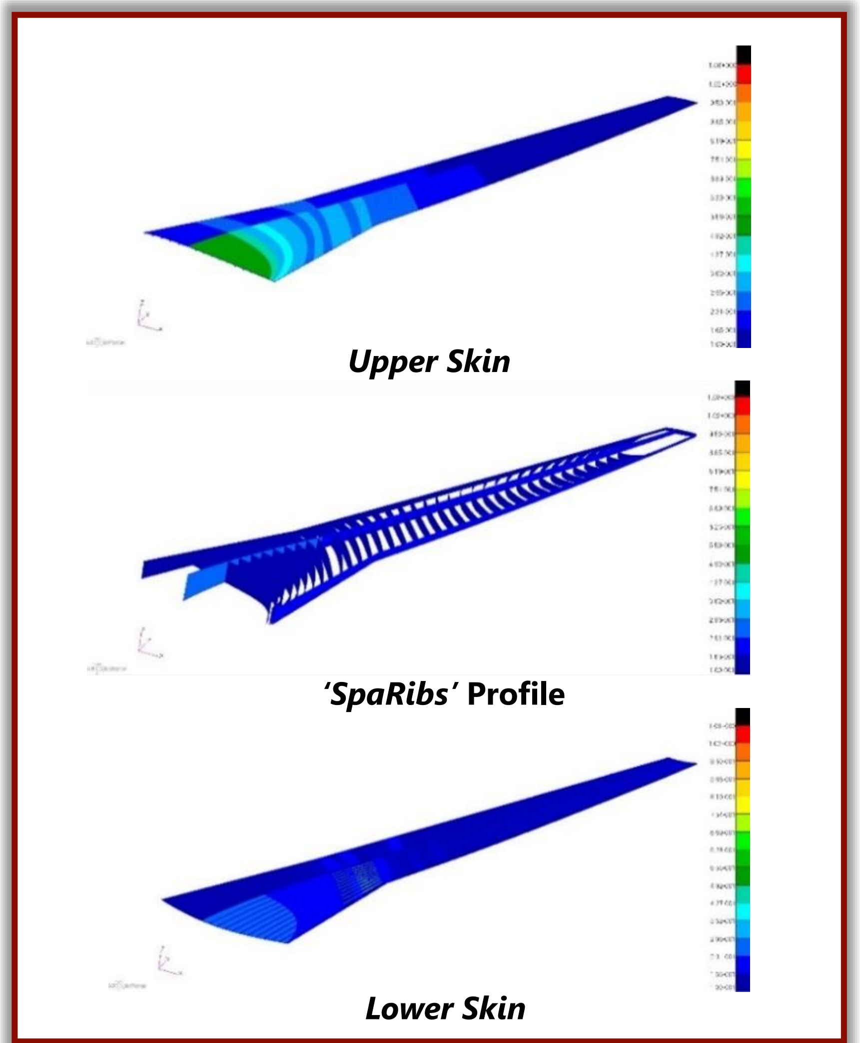


$$\min Obj = f(x, y)$$

A particle swarm searching for the global minimum of a function

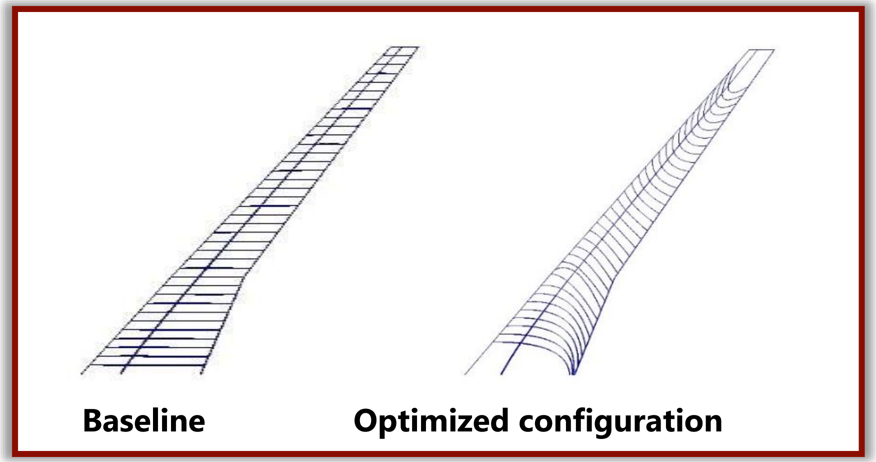
Source: Wikipedia

Optimization Results



Structural Properties for Best Design

Properties	Value
Structural Weight	11002 lb
Total Weight	19102 lb
St. Weight reduction due to SpaRibs	4%
Buckling Factor for AOA 6 degree	1.001 (satisfied)
Buckling Factor for AOA -2 degree	1.05 (satisfied)
Freq. for First Bending Mode	1.29 Hz
Freq. for First Torsional Mode	9.32 Hz
Maximum von Mises Stress	48100 psi (satisfied)
Flutter Velocity (knots)	612 knots (satisfied)



Project Summary

Weight reduction of ~4% achieved for a transport aircraft wing

- Code developed to automate geometry and mesh generation, analysis and optimization for aircraft wing with curvilinear spars and ribs
- Used B-splines to parameterize geometry of curvilinear spars and ribs
- Code written in Python (over 10000 lines!) with parallel computation capability
- Code compatible for Unix Environment
- Multi-level optimization is performed for aircraft wing considering design constraint
- Optimized shape of curvilinear stiffeners to achieve weight reduction

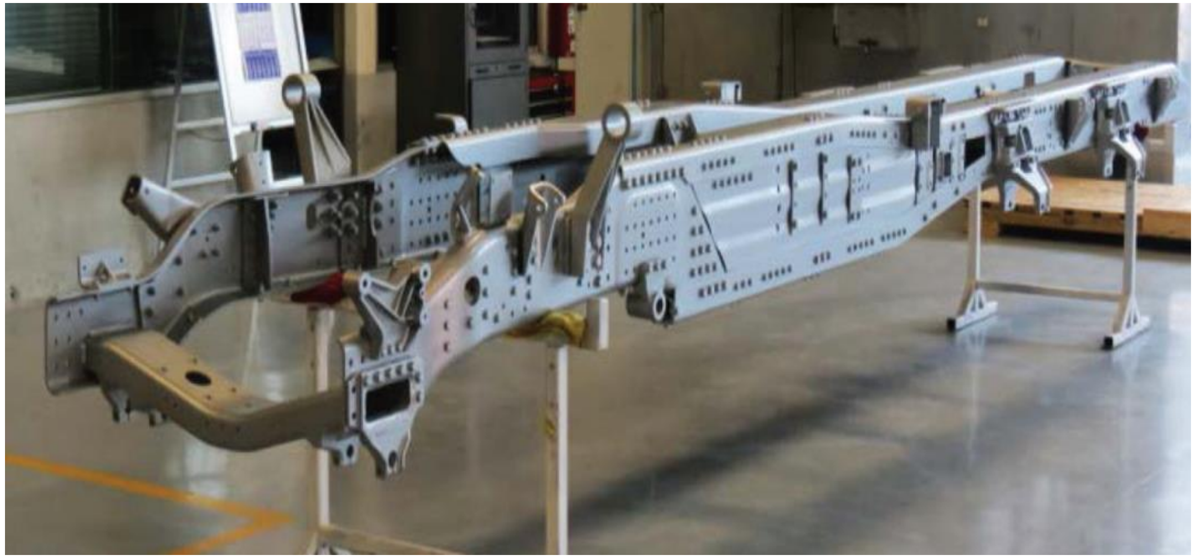
Lightweight Chassis Design for Hybrid Super Trucks

Motivation

Reduce the structural weight of commercial vehicle chassis:

- Highly complex mechanical assembly consisting of side-rail, mountings and several cross-member
- Static analysis corresponding to various road conditions
- Parameterization of geometry using large number of design variables
- Incorporating several constraints – stress, modal frequency and stiffness
- Python script to automate geometry and mesh generation, analysis, evaluation of constraints

Typical Truck Chassis
Photo: Myself



Light-weight Truck chassis prototype
(Source: https://www.energy.gov/sites/prod/files/2014/07/f17/vss081_amar_2014_o.pdf)

Hybrid Truck Chassis Optimization Problem

Goals

- Develop physics based parametric model of truck chassis
- Minimize total Structural Weight of the frame by size and shape optimization
- Use multiple possible road conditions for static analysis (stress computation)

Design Parameters

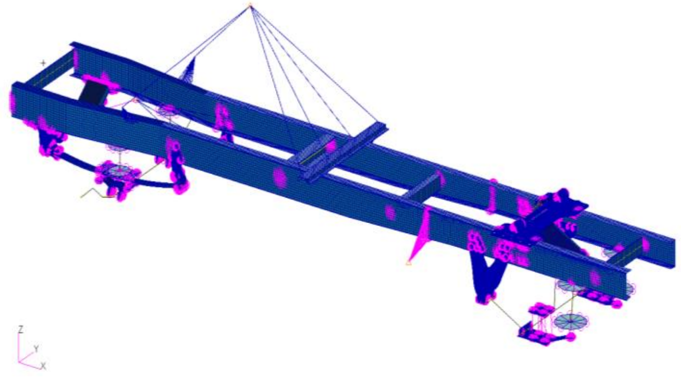
- **Shape Variables**: Defines shape of the rail, internal brackets, hole diameters (range consistent with manufacturing capabilities)
- **Thickness Design Variables**: Thickness of different components (range consistent with available grade of sheet metals)

Constraints

- Violation of von Mises Stress criteria over less than 0.01 % surface area
- Geometric Constraints (e.g., Suspension should attach to the main rail)
- Vertical bending natural frequency > 20 Hz

Note: Due to stress singularities at certain points the maximum von Mises stress is often too high and thus design is based on stress violation factor

Optimization Framework



FEA Model of a Commercial Vehicle Chassis

$$Obj = w + 10^6 \left(\sum max(0, g_i)^2 \right)$$

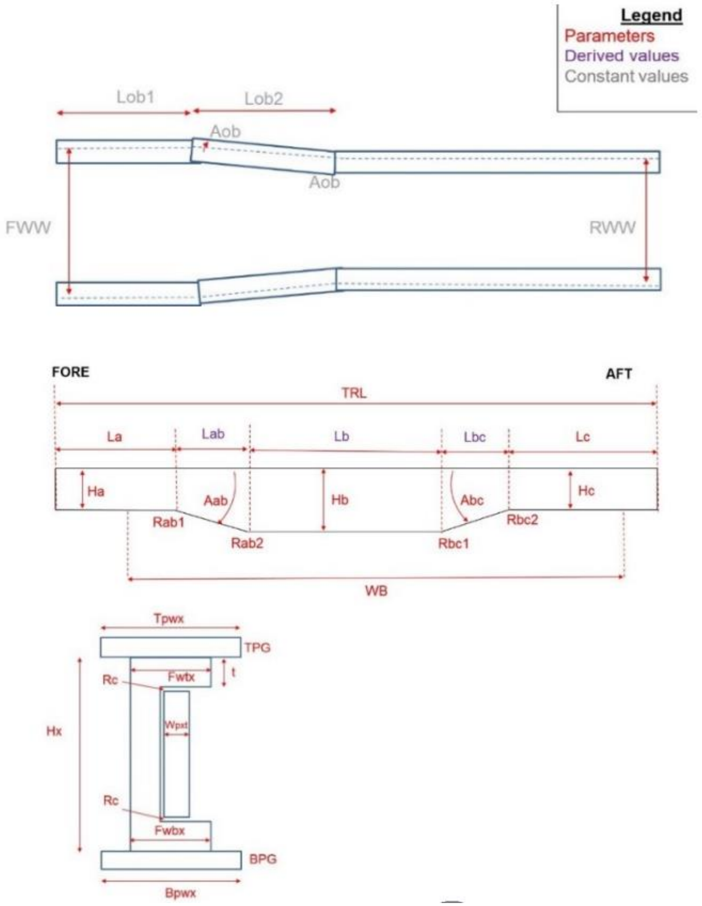
Objective function:

$$g_1 = \frac{Violation}{0.001} - 1$$

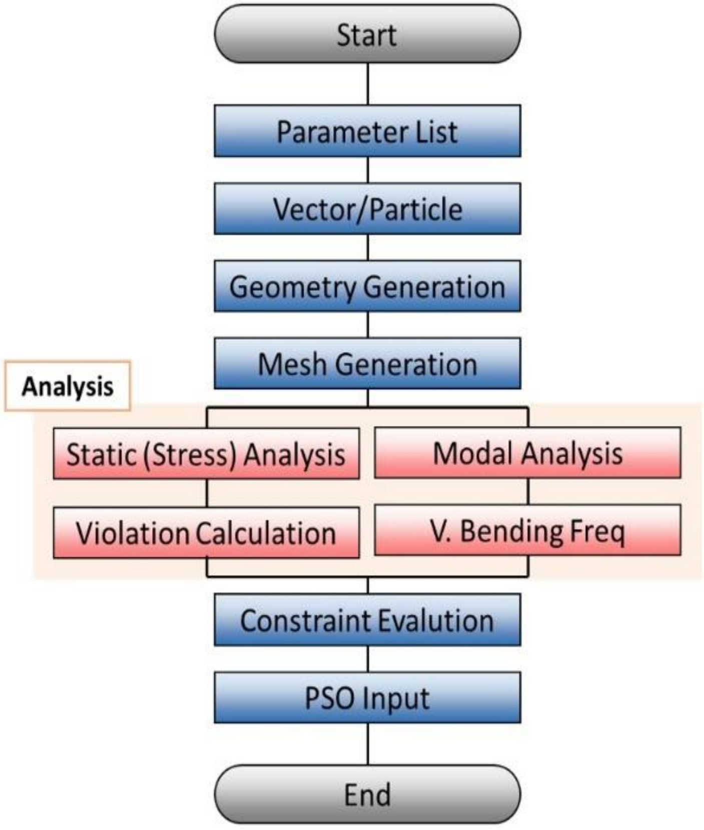
$$g_2 = \frac{f_v}{20} - 1$$

Where:

- Violation is percentage surface area where von Mises stress constraint violated
- W is total weight of frame
- f_v is vertical bending natural frequency



Geometry Parametrization



Code Structure

Frequency Constraint: Modal Assurance Criteria

MAC Function Algorithm

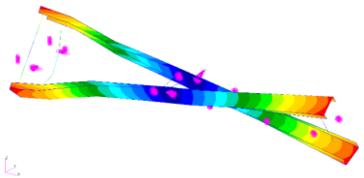
Input — **Mule Chassis Vertical Bending Mode Shapes**

↓

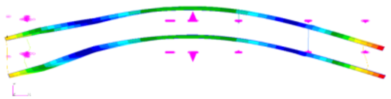
Find the MAC Values for All Testing Mode shapes

↓

Output — **Required Matching Vertical Bending Mode and Natural Frequency**

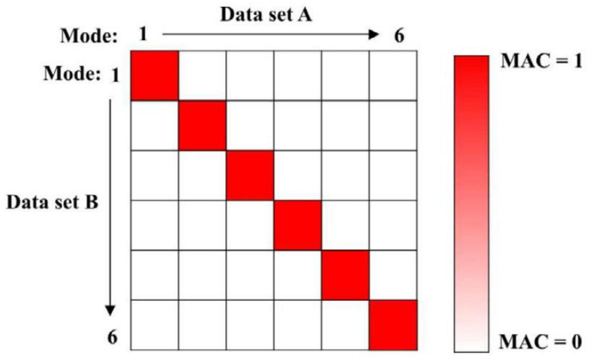


Twisting



Lateral Bending

Vertical Bending



$$MAC = \frac{\left|\{\Phi_A\}^T\{\Phi_B\}\right|^2}{(\{\Phi_A\}^T\{\Phi_A\})(\{\Phi_B\}^T\{\Phi_B\})}$$

Mule Model (Reference: A)

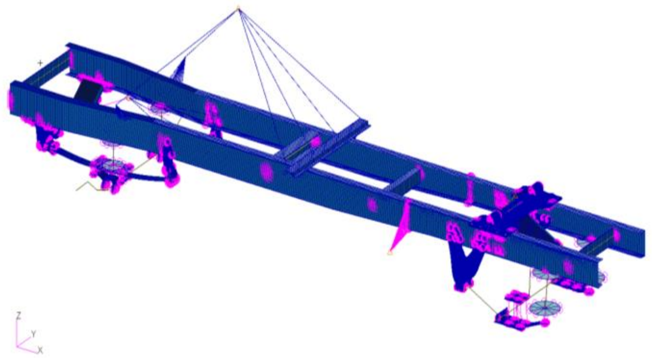
Random Test Model (B)

Natural Freq: [3.969, 10.57, 22.23, 25.43, 26.14, 27.313, 30.08, **31.94**, 33.63]

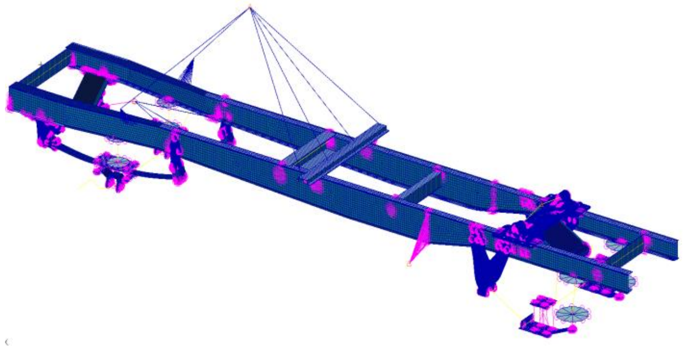
MAC: [3.5e-08, 4.9e-07, 4.4e-05, 8.9e-2, 2e-3, 2.3e-05, 3.2e-05, **0.4**, 3e-3]

Optimization Results

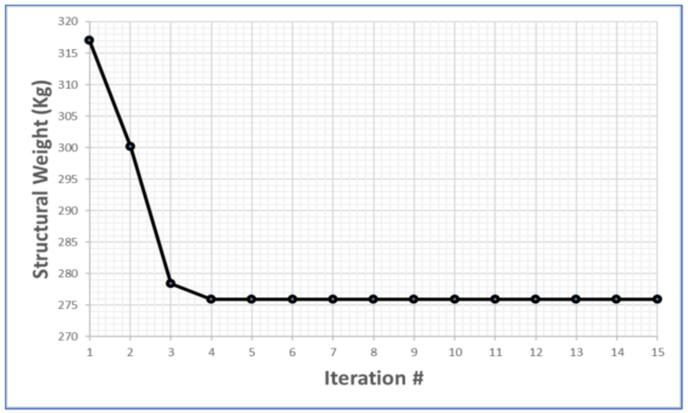
- Optimized design has mass 275 Kg (13.25% less than baseline design)
- Vertical bending frequency and max Violation 20.5 Hz and 0.0086, respectively (close to constraint values)

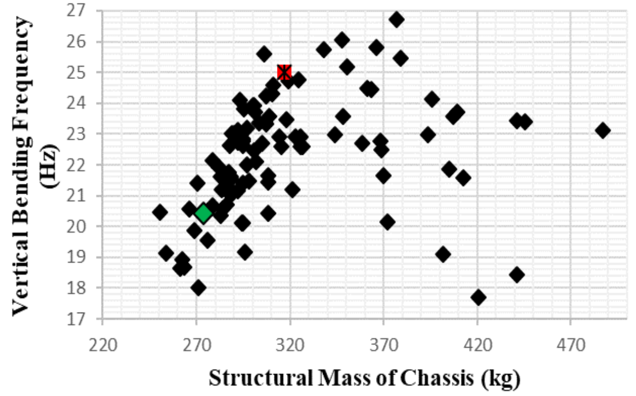


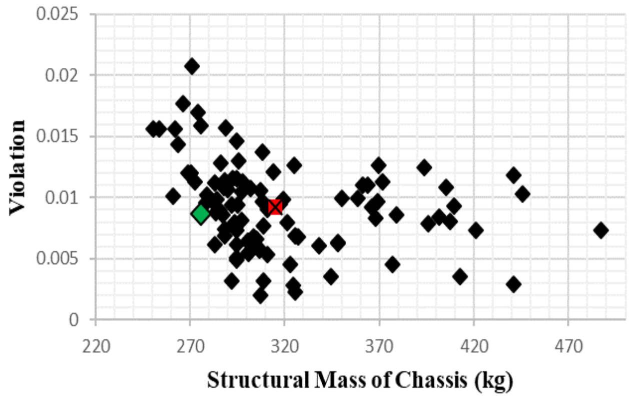
Baseline



Optimized Design



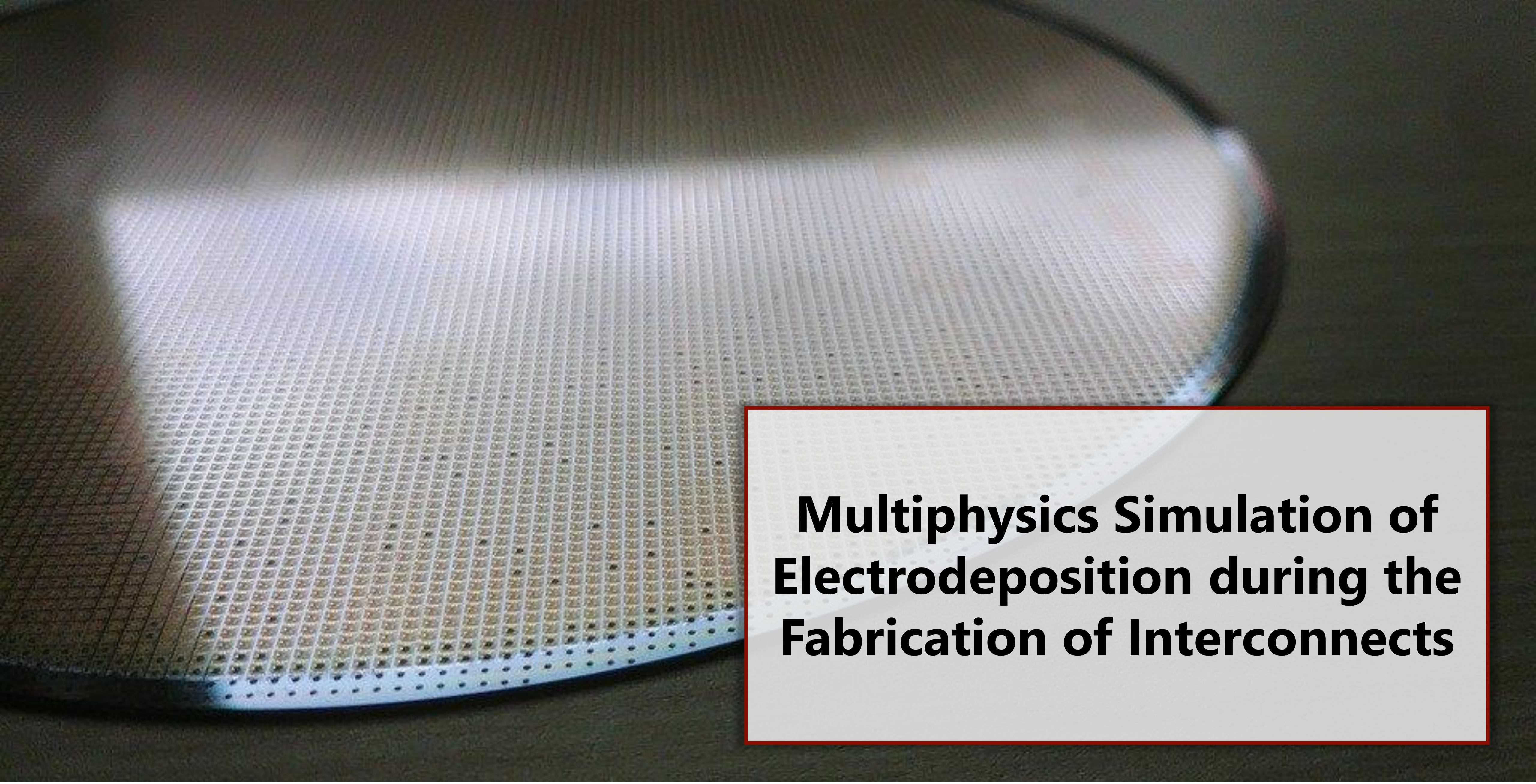




Project Summary

Size and shape optimization achieved a 13.25% weight reduction

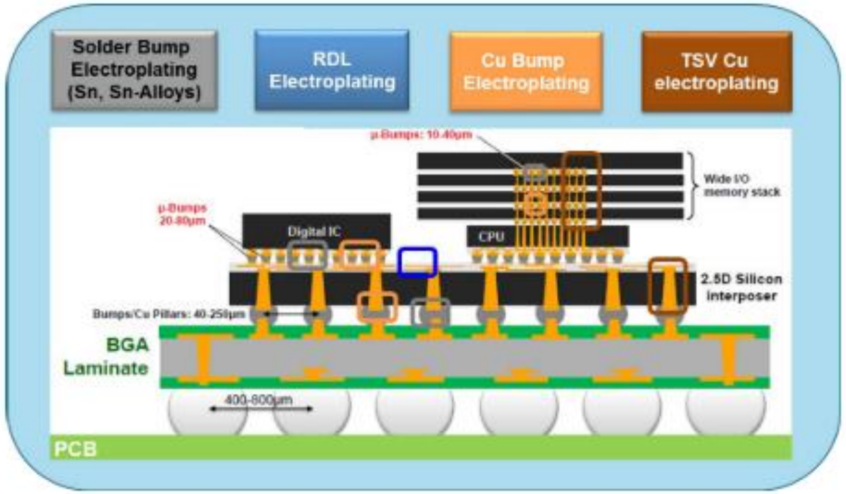
- Code developed to automate geometry and mesh generation, analysis for complex chassis geometry
- Optimization Side rail parameterization with 30 design variables (size and shape)
- Modal Assurance Criteria used to determine the first vertical bending frequency
- Integration of elements such as front and rear suspension to form a complete model
- Performed structural optimization for automotive chassis
- Accomplished comprehensive non-linear static analysis of vehicle suspension (experimental validation)
- Verified low-fidelity model with high-fidelity results



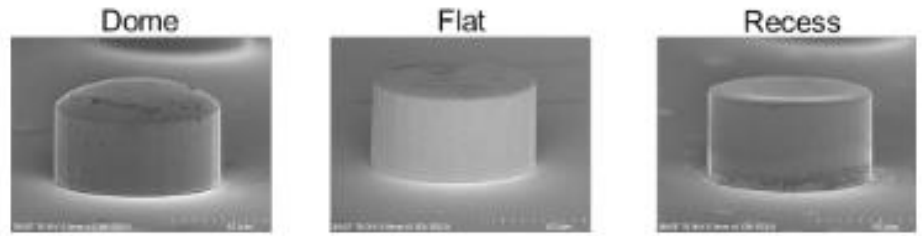
Multiphysics Simulation of Electrodeposition during the Fabrication of Interconnects

Motivation

- Manufacturing of interconnects in packaging of integrated circuits are usually achieved by electrodeposition of Cu and other metals in micro-nano holes with fluid flow
- Organic additives (which modifies the current) applied to obtain defect-free "flat" deposition
- Challenging to find appropriate organic additives
- Simulation of the process using Finite Element Methods can expedite the research and development
- Process simulation / prediction requires determination of kinetic parameters (of Cu and additives)



Copper Packaging (Source: BASF)



Different Copper Micro Bumps due to fluid flow and additives (Source: BASF)

Kinetic Parameter Estimation

System

- 1-D
- Steady state
- Rotating disc electrode (vicinity surface)
- Use Tafel equation for kinetic approximation

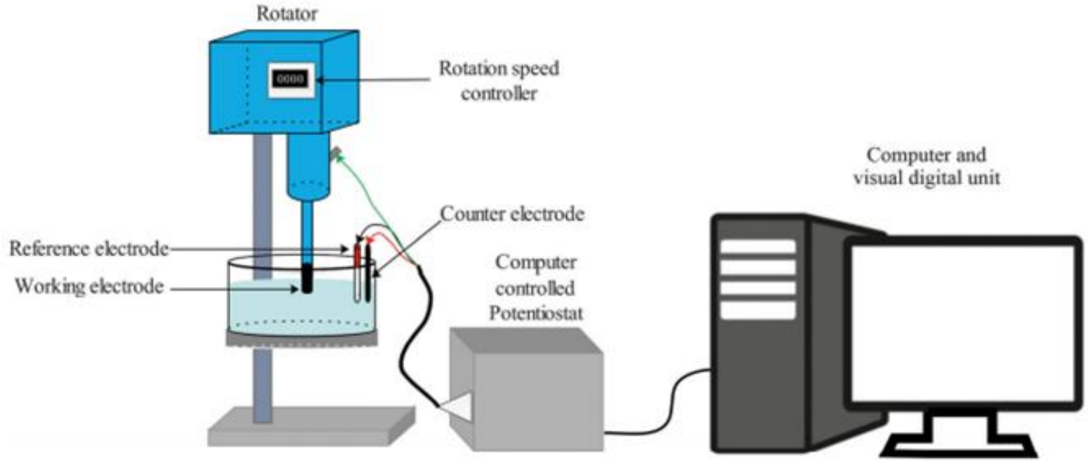
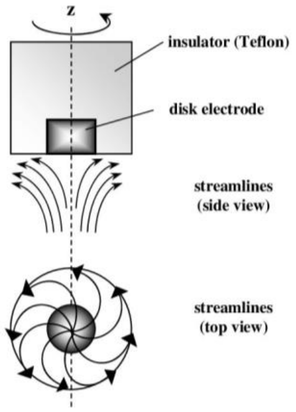
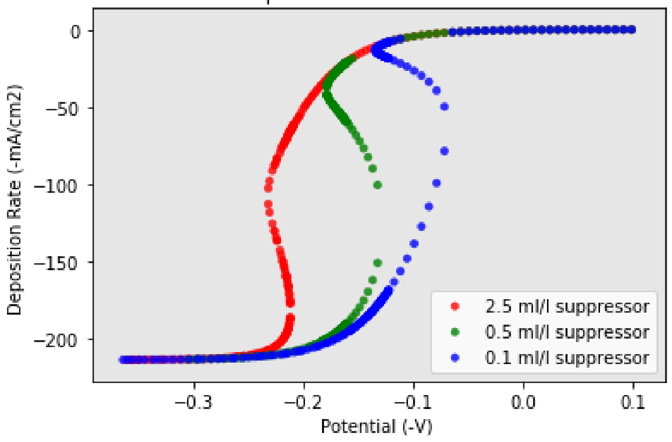


Figure 1. Schematic of the rotating disc electrode setup for the electrochemical measurements.
Credit: https://doi.org/10.1080/00032719.2019.1700515



Rotating Disc Electrode Cathode



LSV Curve recorded

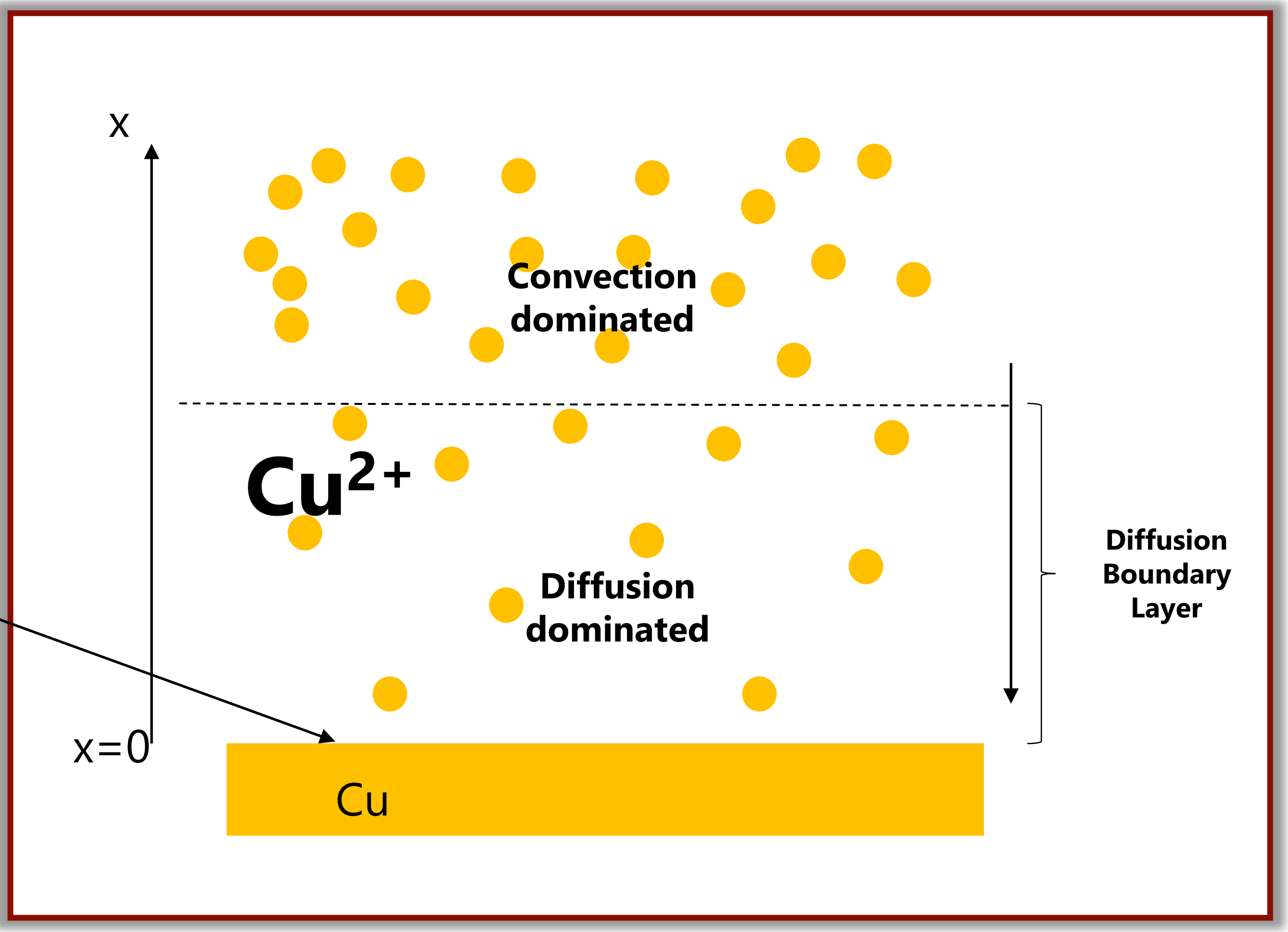
Physiochemical Model (Cu without additives)

- Tafel equation is used for cathodic deposition only
- Applicable for RDE and 1D geometry

$$Cu^{2+} + 2\,e \rightarrow Cu$$

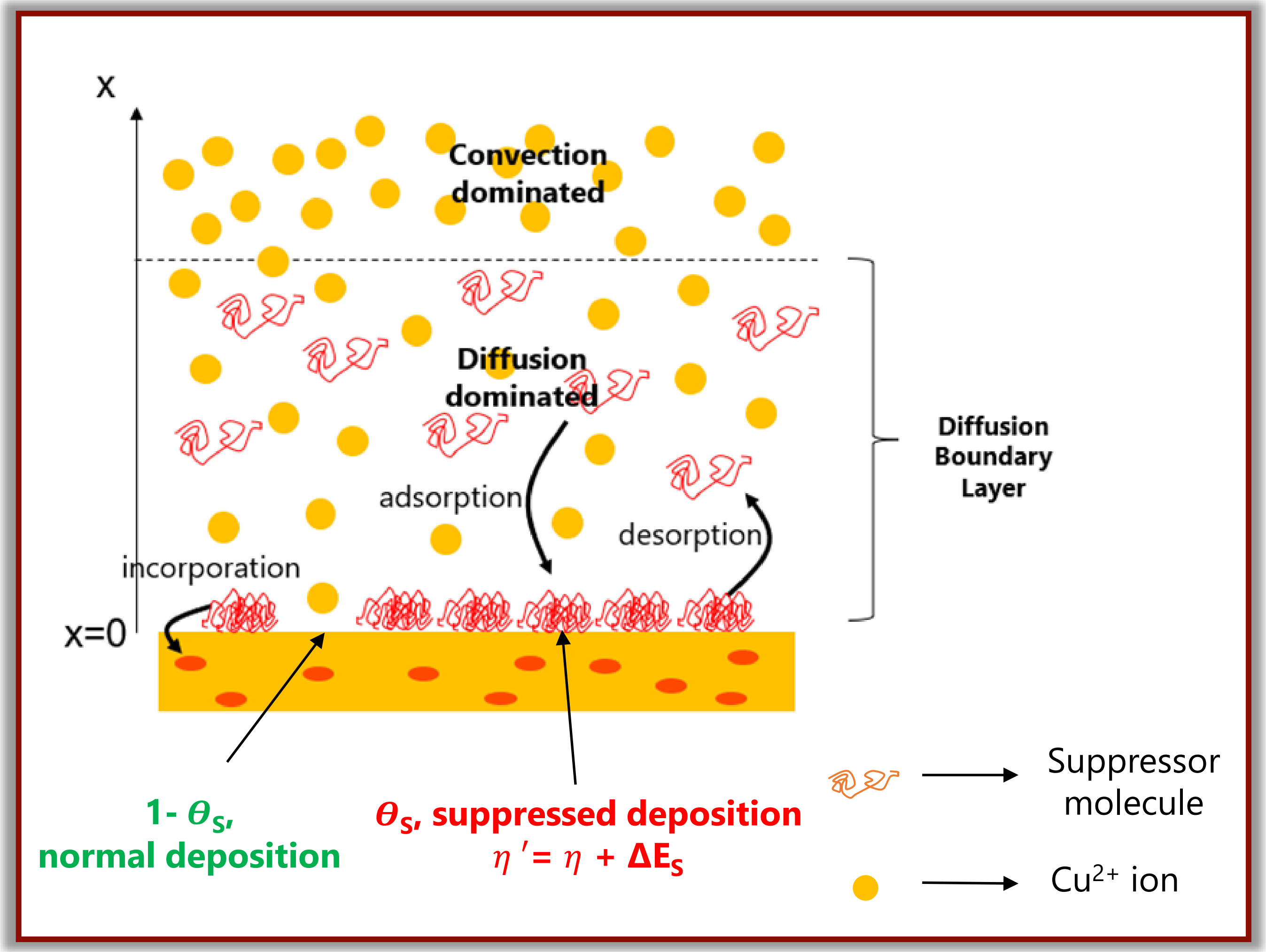
$$r = k_{Cu} \cdot exp(-b_{Cu} \cdot \eta) \cdot C_{Cu^{2+},x=0}$$

k_{Cu} : Reaction rate constant
b_{Cu} : Tafel slope
η : Over potential for deposition (after the correction of ohmic drop)



Physiochemical Model (with Suppressor)

- Cu deposition on additive free surface fraction remains unchanged.
- Cu deposition on suppressor covered surface shifts by a constant over potential, ΔE_S.
- θ_S is fractional surface coverage of suppressor on surface



Numerical Model

Governing Differential Equation (steady state):

$$\frac{d^2C_{Cu}}{dx^2} - \frac{V}{D_{Cu}}\frac{dC_{Cu}}{dx} = 0$$

$$\frac{d^2C_s}{dx^2} - \frac{V}{D_S}\frac{dC_s}{dx} = 0$$

$$V = -0.51023\,\omega^{\frac{3}{2}}\,v^{\frac{-1}{2}}x^2$$

$C_{Cu}{}^*$: Cu concentration at infinity

$C_S *$: Suppressor concentration at infinity

V : Velocity function of fluid

Boundary conditions:

$$@\ x = 0\ ,D_{Cu}\frac{\boldsymbol{dC_{Cu}}}{\boldsymbol{dx}} = A_{Cu}(1-\Theta_S)\ C_{Cu}$$

$$@\ x = \infty,\ C_{Cu}{=}C_{Cu}{}^*$$

$$@\ x = 0\ ,D_S\frac{\boldsymbol{dC_s}}{\boldsymbol{dx}} = A_{S,AD}(1-\Theta_S)\ C_S\ - \Theta_S A_{S,D}$$

$$@\ x = \infty,\ C_S{=}C_S *$$

Adsorption = *Desorption* + *Consumption*

$$@\ x = 0\ ,\ \ C_s(1-\Theta_S)A_{S,AD} = A_{S,D}\Theta_S + A_\theta\Theta_S A_{Cu}C_{Cu}\,(1-\Theta_{eq})$$

$$A_{Cu} = k_{Cu}\ e^{-b_{Cu}\eta}$$

$$\eta\,' = \eta + \boldsymbol{\Delta}\mathrm{E_S}$$

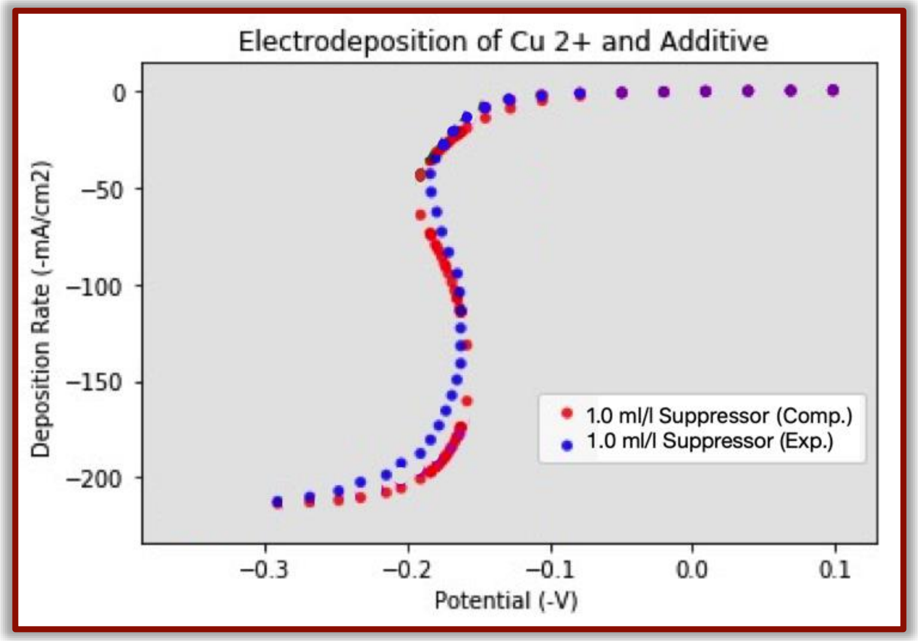
$$A_{S,D} = k_{S,D}e^{-b_{S,D}\eta}$$

$$A_{S,AD} = k_{S,AD}\ e^{-b_{S,AD}\eta}$$

$$A_\theta = k_\theta\ e^{-b_\theta\eta}$$

Fitting Experimental and Theoretical CV Curves

- k_{Cu} and b_{Cu} used as obtained form fitting Cu-case
- $k_{S,D}$, $b_{S,D}$, $k_{S,AD}$, $b_{S,AD}$, k_{θ} , b_{θ} are design variables
- Experimental curves may or may not show NDR region (depending on additive concentration)
- k_{Cu}, b_{Cu} considered design variable
- Objective function is **sum of square of difference** between experimental and theoretical current over the range of voltage
- Particle Swarm Optimization (PSO) applied to minimize Objective function
- Convergence achieved when Obj function didn't change for several iterations



Fitting exp and theoretical CV curves

$$A_{Cu} = k_{Cu}\ e^{-b_{Cu}\eta}$$
$$A_{S,D} = k_{S,D} e^{-b_{S,D}\eta}$$
$$A_{S,AD} = k_{S,AD}\ e^{-b_{S,AD}\eta}$$
$$A_{\theta} = k_{\theta}\ e^{-b_{\theta}\eta}$$

Simulation of Cu Bump Plating - Method

- A python script is developed involving COMSOL and MATLAB Livelink to run quasi-static analysis of electrodeposition including multiple additives
- COMSOL solves coupled Navier-stokes Equation (hydrodynamics) and Nernst-Plank Equation (electrochemistry) for each time step
- Both potentiostatic (constant potential difference) and galvanostatic (constraint current) analysis can be performed
- All parameters to describe various elements such as geometry, time-step size, additive dosage, flow velocity and others need to be provided as input
- The surface-coverage is updated after every time-step (involving kinetic parameters of additives, surface concentration of additives, surface-coverages in the previous timestep)
- Simulation continues till the maximum number of timestep reached (or the hole is filled)

Simulation of Cu Bump Plating - Model

Navier-Stokes Equation(Solved using COMSOL)

$\boldsymbol{\rho}$, **u**, $\boldsymbol{\mu}$ **=** Density, Fluid velocity, Viscosity

$$\rho\frac{\partial \boldsymbol{u}}{\partial t} + \rho(\boldsymbol{u}.\nabla \boldsymbol{u}) = \nabla[-p\boldsymbol{I} + \mu(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T]$$

$$\rho(\nabla.\boldsymbol{u})=0$$

Nernst-Plank Equation (Solved using COMSOL)

$\boldsymbol{F}$, **R**, **T**, $\boldsymbol{\varphi}$ **=** Faraday, Gas constant, Temperature, Electric potential field

$\boldsymbol{D_i}$, $\boldsymbol{c_i}$, $\boldsymbol{z_i}$ **=** Diffusion Coefficient, Concentration, valance of i[th] ionic species

$$\frac{\partial c_i}{\partial t} = -\nabla.J$$

$$J = -D_i[\nabla c_i + \frac{z_i F}{RT}c_i(\nabla\varphi)]$$

Mass balance of surface coverage at cathode surface (additive cases) (solved by Python script)

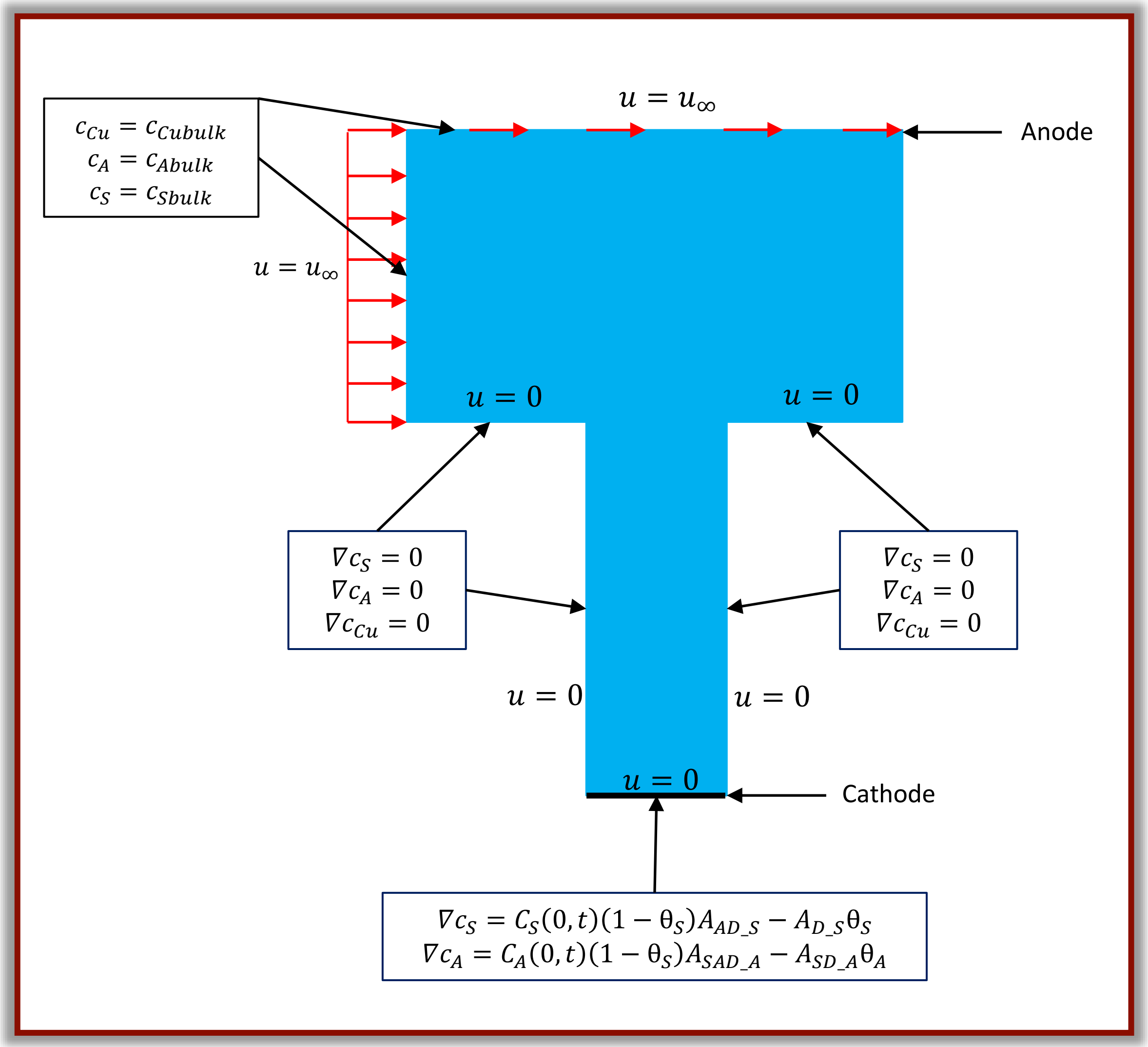
Change of the coverage = Adsorption – Desorption – Consumption

$$\frac{d\theta_S}{dt} = K_{molecule\_S}\cdot\{C_S(0,t)(1-\theta_S-\theta_L)A_{AD\_S} - A_{D\_S}\theta_S - A_{\theta\_S}A_{Cu}C_{Cu}(0,t)\theta_S(1-\theta_{eq})\}$$

$$\frac{d\theta_A}{dt} = K_{molecule\_A}\cdot\{C_A(0,t)(1-\theta_A)A_{AD\_A} - A_{D\_A}\theta_A - A_{\theta\_A}A_{Cu}C_{Cu}(0,t)\theta_A(1-\theta_{eq})\}$$

$$\frac{d\theta_L}{dt} = K_{molecule\_L}\cdot\{C_L(0,t)(1-\theta_S-\theta_L)A_{AD\_L} - A_{D\_L}\theta_L - A_{\theta\_L}A_{Cu}C_{Cu}(0,t)\theta_L(1-\theta_{eq})\}$$

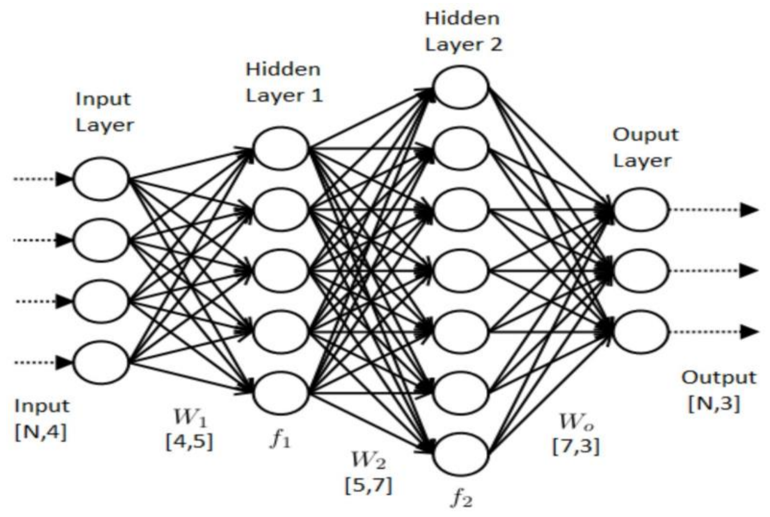
$$\theta_{eq} = f(\theta_S, \theta_L, \theta_A)$$



Machine Learning Implementation

- The idea is to train a “black-box” function to relate input and output when the physics is not understood or difficult to assess
- Multiphysics Simulation is computationally expensive
- It is convenient to use Deep Learning to predict quality of deposition for given parameters

- **Deep Learning Implementation:**
  - Model generated using randomized parameters
  - Each simulated profile labelled from 1-10 (according to quality)
  - Data classified into “Training set”, “Dev set” and “Test set”
  - Neural network trained and tested using that data
  - Hyperparameter tuning is being carried out



Neural Network Architecture

Project Summary

Proficiently presented the change in micro-bump profile simulation due to the addition of additives

- COMSOL used for Multiphysics model of Cu deposition in micro bump involving additives
- Used additive properties by fitting experimental LCV curves
- Flexible model which can considers large number of environmental factors
- Change in deposition profile due to additives demonstrated
- Deep Learning Algorithm trained for predicting deposition quality given kinetic parameters

Conclusion

- Finite Element Method (FEM) is a numerical technique to solve complex differential equation popular in science and engineering
- Projects described to demonstrate application of FEM in aerospace, automobile and chemical engineering
    - Bio-inspired aircraft wing design and optimization
    - Light-weight truck chassis design for hybrid super trucks
    - Manufacturing of defect-free interconnects using organic additives
- The projects involve python scripting to streamline the process of geometry generation, mesh generation, analysis, optimization and postprocessing
- FEM is constantly improved to describe more complex physics (including non-linear biological phenomenon)

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