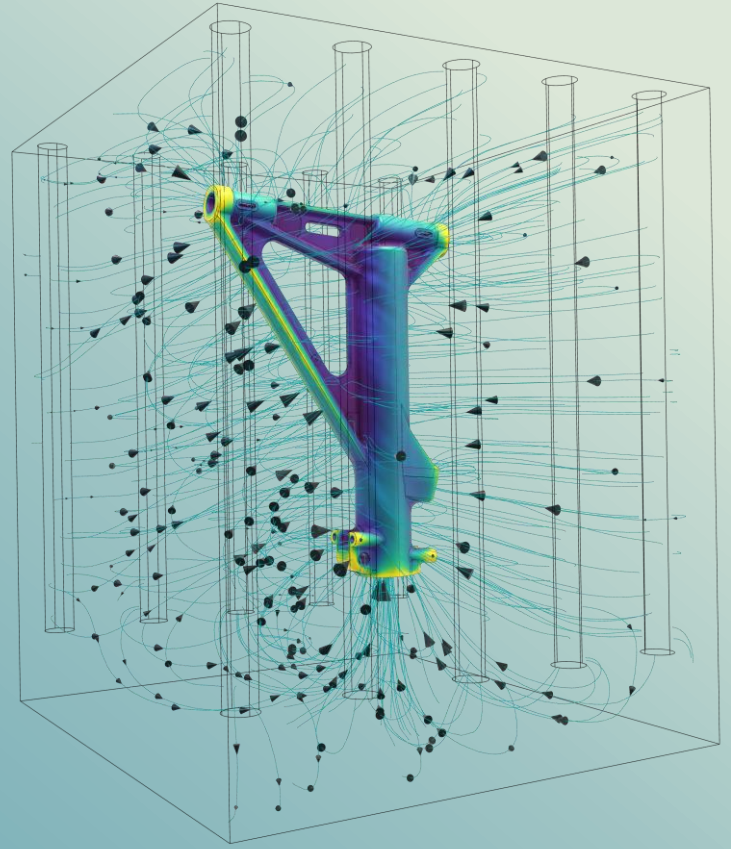
HIVELIX

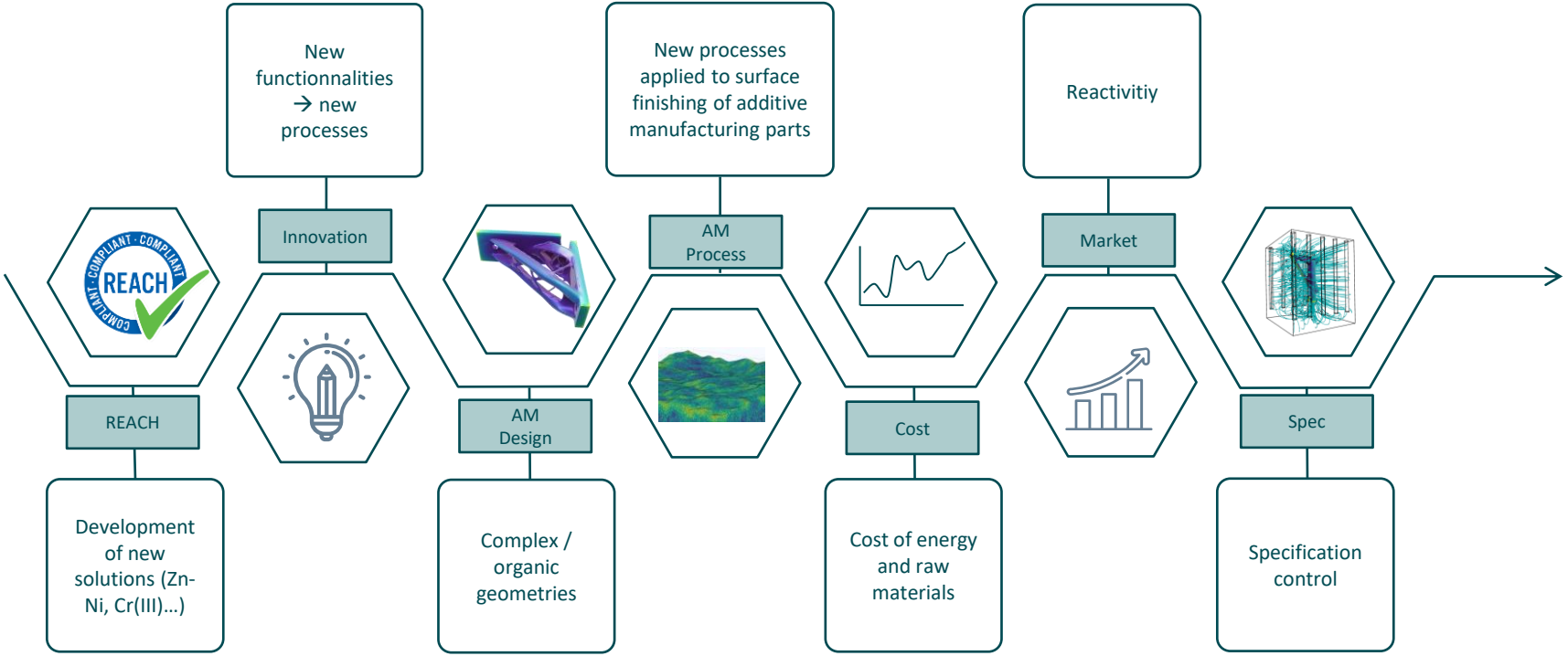
# OPTIMISATION DES PROCÉDÉS DE FINITION DE SURFACE : SYNERGIE ENTRE SIMULATION MULTI ÉCHELLE, MULTIPHYSIQUE ET MACHINE LEARNING

## OPTIMIZATION OF SURFACE FINISHING PROCESSES: SYNERGY BETWEEN MULTI-SCALE, MULTIPHYSICS SIMULATION AND MACHINE LEARNING



Mécamat 2024

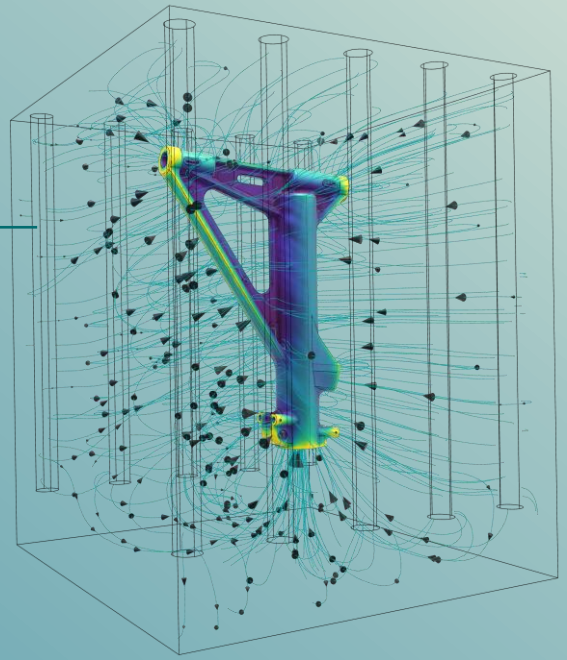
# SURFACE FINISHING INDUSTRY MARKET




Surface finishing industries need to integrate digitalization in order to reduce costs from empirical approaches, support innovation, and reduce raw material consumption

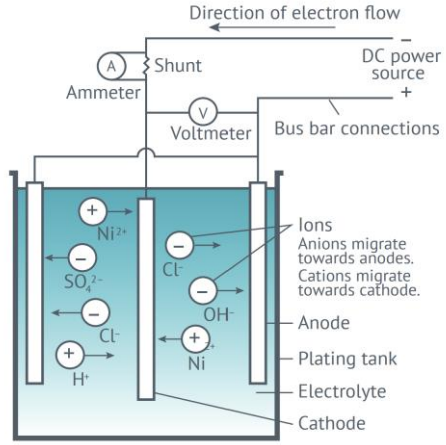
# MULTIPHYSICS AND MULTISCALE MODELING

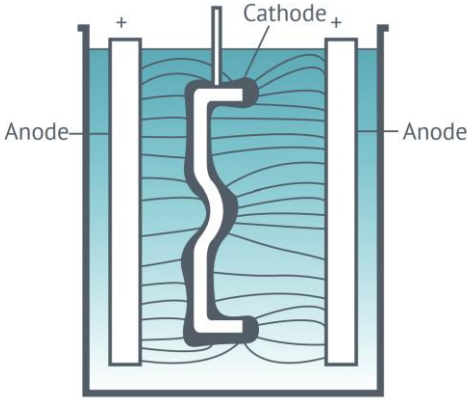
MULTIPHYSICS MODELING



# CONTEXT

- The development of new electrolytes in electrolytic coatings has been driven by REACH environmental regulations since several years :
  - Zinc-nickel substitution for cadmium
  - Substitution of hexavalent chromium by trivalent chromium…
- In the case of zinc-nickel electrolytic coatings, used for their anti-corrosion properties, it is necessary to maintain specifications on complex parts such as :
  - Thickness distribution, with more or less tolerance depending on requirements
  - Composition, to be stabilized between 12% and 16% to ensure the best anti-corrosion performance
- Good control of process parameters and industrial electrochemical cell sizing is essential to maintain these specifications on a complex part
- Electrochemical processes are intrinsically heterogeneous due to the distribution of current within an electrochemical cell, as can be seen in cases such as electroplating, anodizing and electropolishing....
- Current distribution and the local efficiency depend on many parameters, including process parameters (applied current, process duration, temperature, etc.), electrolyte chemistry and associated properties (conductivity, viscosity, pH, etc.), and fluid flow (mass transport, local concentration)




Nickel plating handbook – Nickel Institute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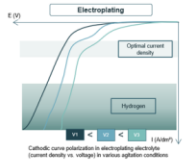
# MULTIPHYSICS AND MULTISCALE MODELING OF SURFACE FINISHING PROCESSES

**Define physics assumptions and study scale**
- Current distribution mode? Hydrogen evolution? Hydrodynamics? Double layer evolution? Nucleation phenomenon...

**Behaviour law definition**
- Experimental caracterisation of electrode kinectics

$$i_{loc,Cu} = i_{0,Cu}\left(exp\left(\frac{\alpha_a \cdot F \cdot \eta_{Cu}}{R \cdot T}\right) - exp\left(\frac{-\alpha_c \cdot F \cdot \eta_{Cu}}{R \cdot T}\right)\right)$$

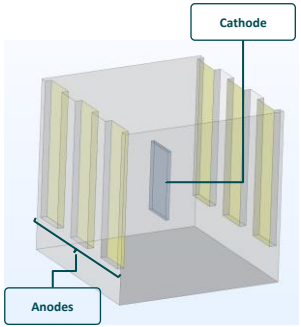


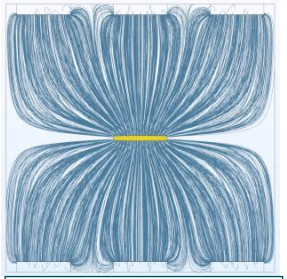
Cathodic curve polarization in electroplating electrolyte (current density vs. voltage) in various agitation conditions

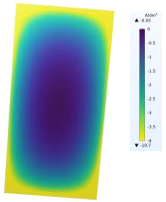
**CAD and Mesh**

**Resolve equations**

**Explore results**
- Thickness
- Current density
- Alloy composition





Current lines
Top view


Local current density

How to maintain coating specifications on complex parts ?

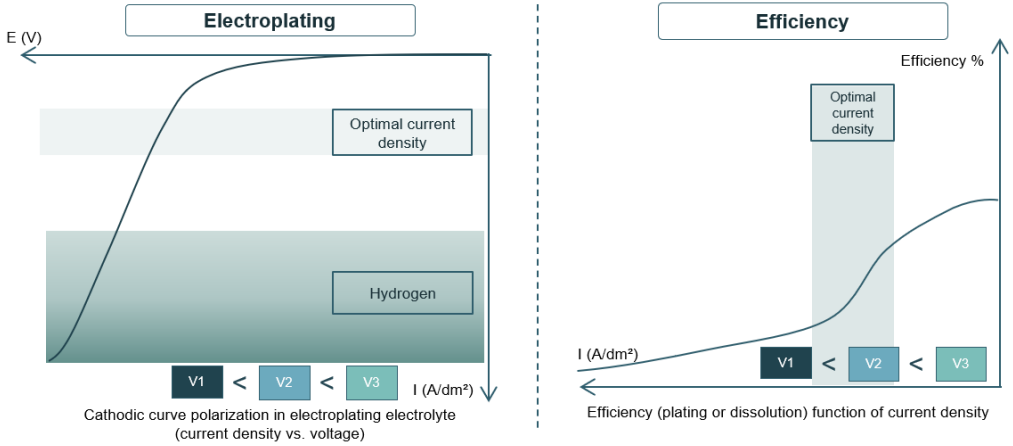
# MULTIPHYSICS AND MULTISCALE MODELING OF SURFACE FINISHING PROCESSES

- Electroplated coating quality (thickness, composition, properties, etc.) depends on the ability to maintain a uniform current distribution and efficiency across all treated parts, as well as to replenish beneficial species (ions, additives, etc.) and eliminate harmful species (such as hydrogen) during the electroplating process
- Each electrolyte has its own operating range and robustness against process parameters driven by its electrochemical kinetics
- Mass transport is driven by several contributions :
  - Diffusion ( Fick laws)
  - Migration (Nernst Law)
  - Convection (Navier-Stokes)

1 (Nernst-Planck) $\frac{\partial n_i}{\partial t} = \nabla \cdot [D_i \nabla n_i + \mu_i n_i \nabla \phi - n_i \mathbf{u}]$ (diffusion, migration, convection)

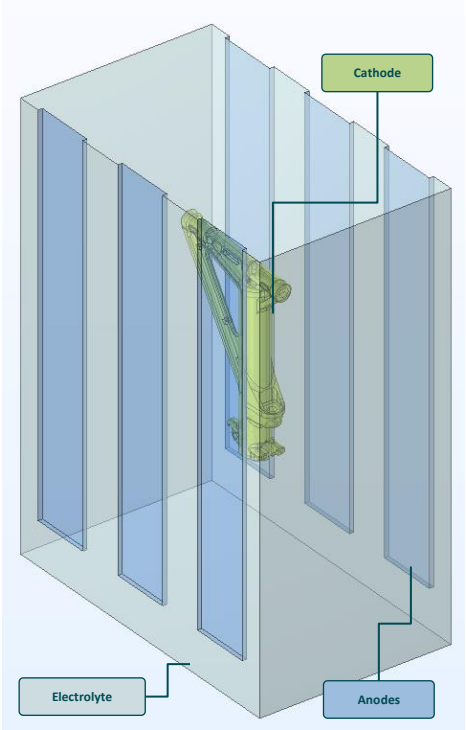
$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) = -\nabla p + \eta \nabla^2 \mathbf{u} - \nabla \phi \sum_{i=1}^{N} z_i e n_i \quad \Longleftrightarrow \quad \nabla^2 \phi = -\frac{1}{\epsilon \epsilon_0} \sum_{i=1}^{N} z_i e n_i$$

$\nabla \cdot \mathbf{u} = 0$ (Navier-Stokes) (Poisson)




Cathodic curve polarization in electroplating electrolyte (current density vs. voltage)

Efficiency (plating or dissolution) function of current density





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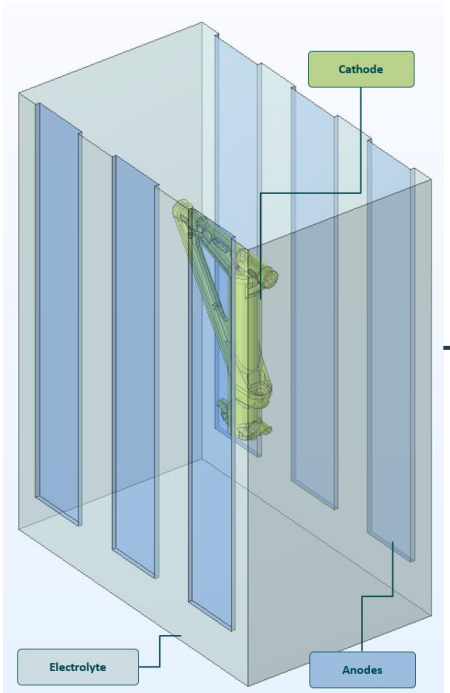
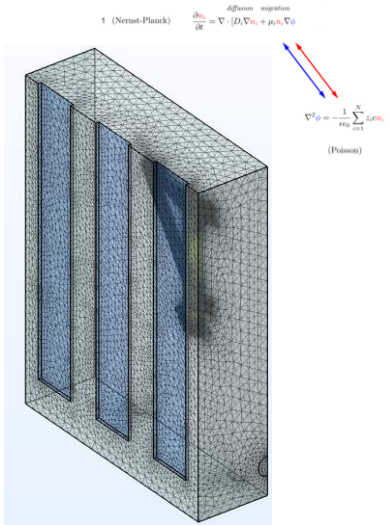
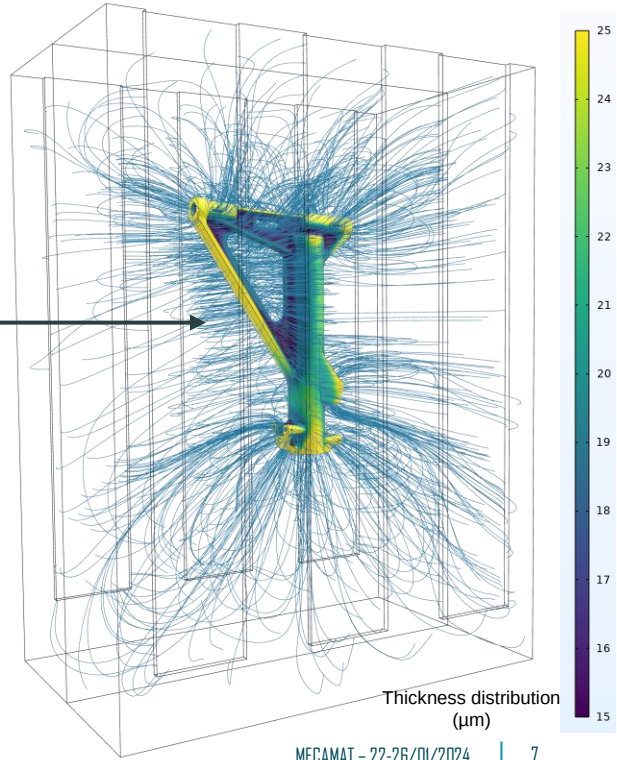
# MULTIPHYSICS AND MULTISCALE MODELING OF SURFACE FINISHING PROCESSES

- In the case of complex geometries such as these, electrolyte throwing power is a problem, resulting in heterogeneous processing. Under-thicknesses appear in hollow bodies. In addition, over-thicknesses can be observed at the edges
- Throwing power is a critical parameter in electroplating, essentially describes the electrolyte's ability to ensure uniform deposition, particularly in recessed areas. Given the complexity of the geometry, it is essential to optimize penetration power using specific tooling




**Simulation only with secondary current distribution model**




Thickness distribution (µm)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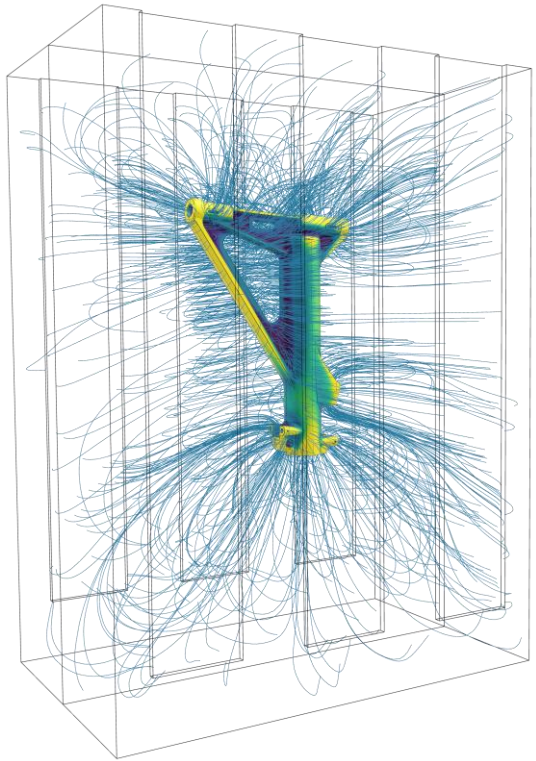

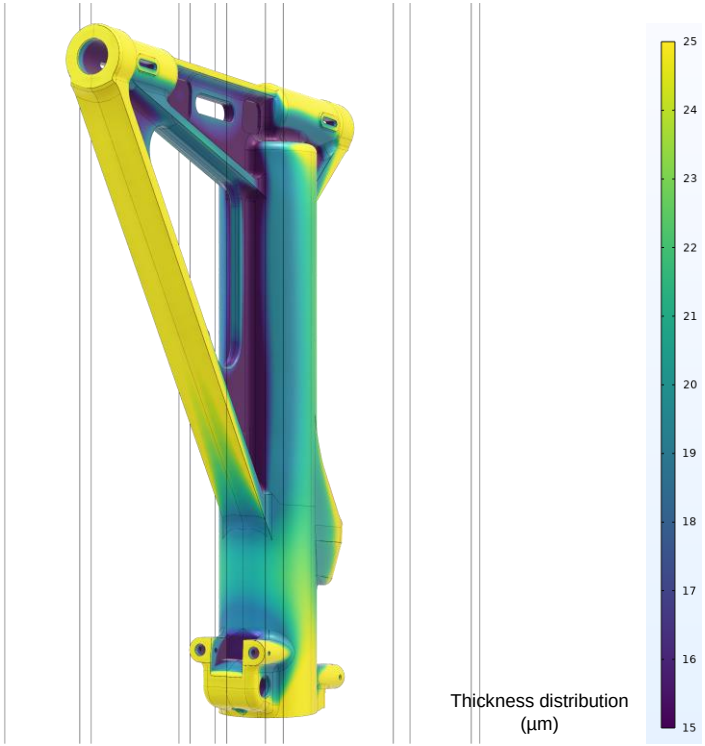


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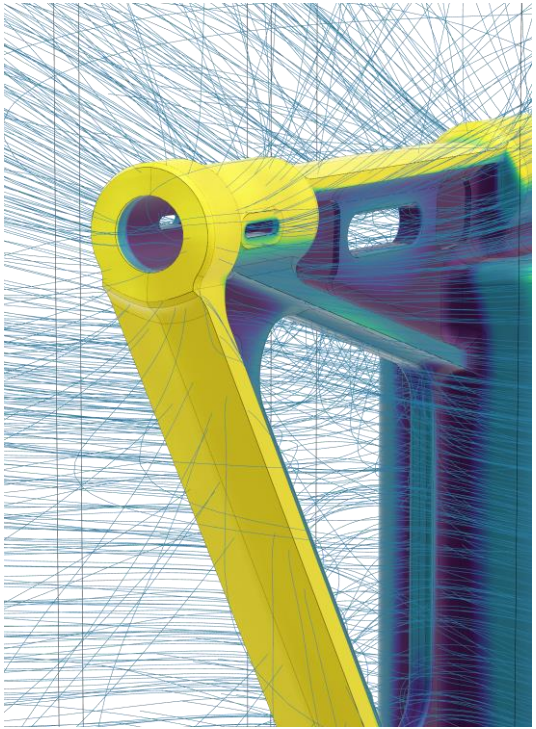
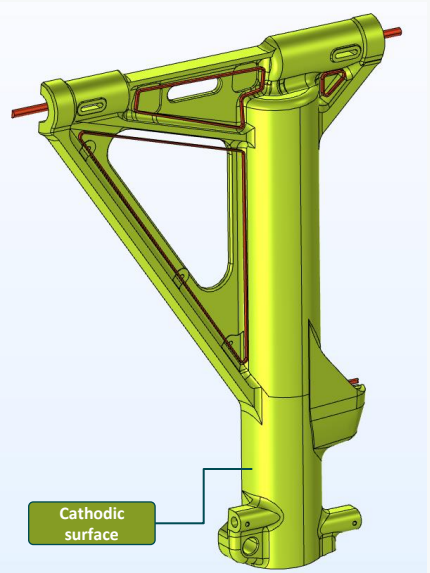
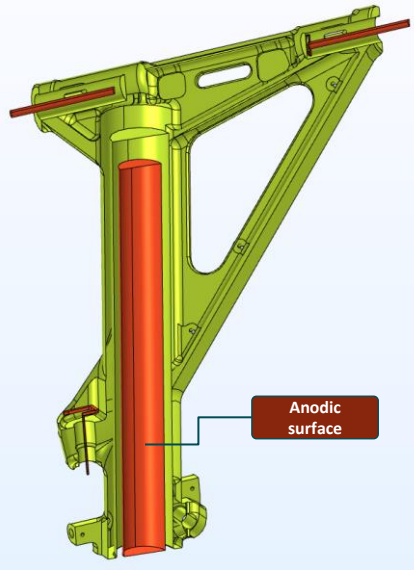


Additional auxiliary anodes, managed by a main generator or an external generator, improve current distribution over the whole part.





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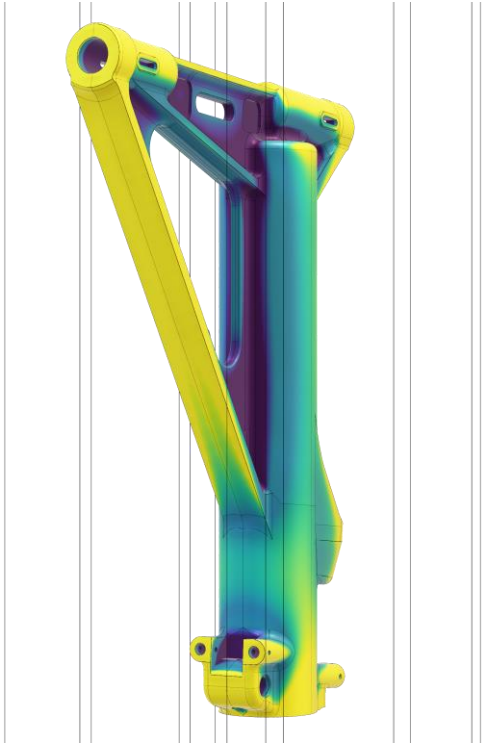
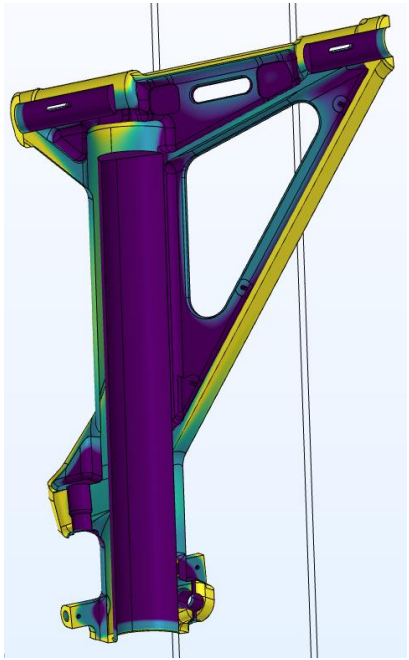
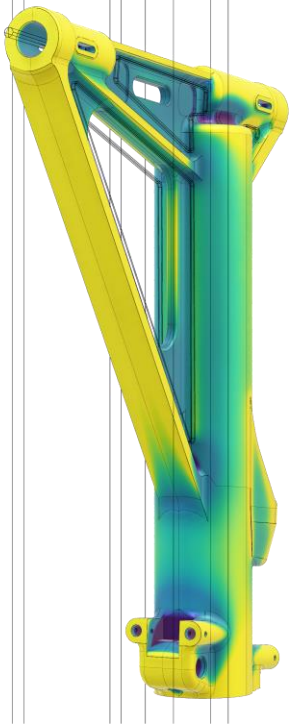
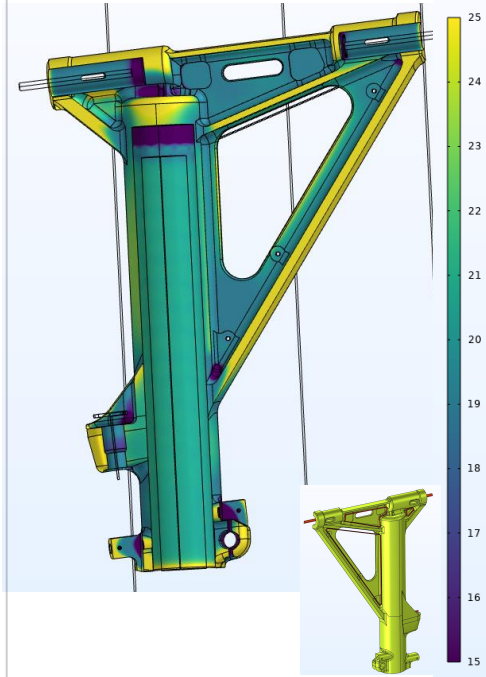




Thickness distribution (µm)







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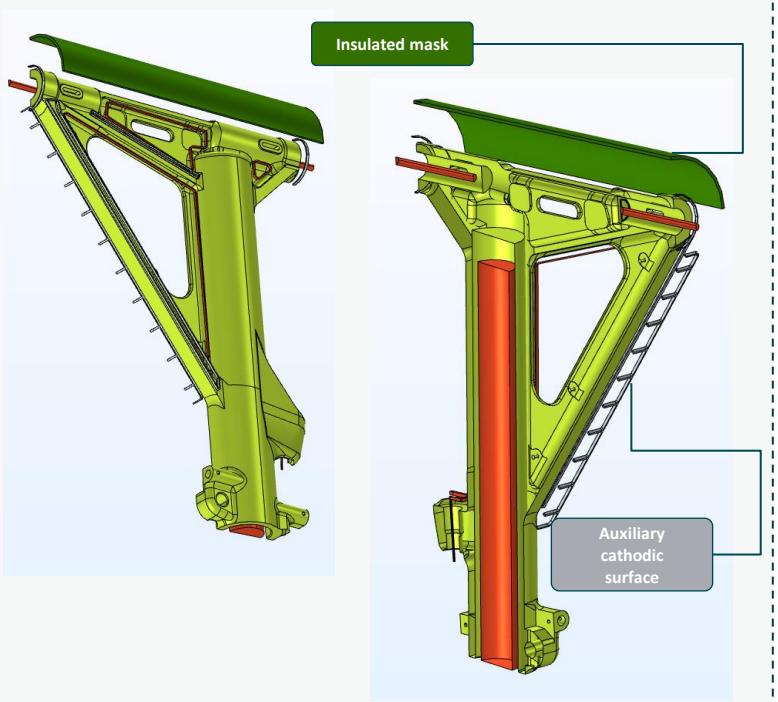
Additional auxiliary anodes, managed by a main generator or an external generator, improve current distribution over the whole part.

Current robber and isolated mask can also improve thickness distribution





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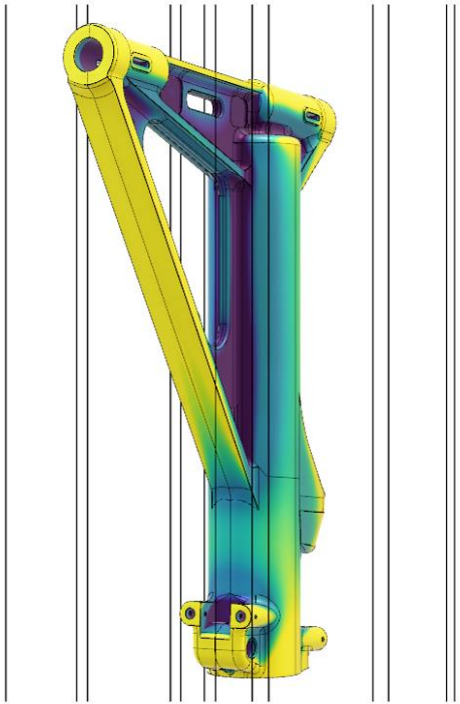
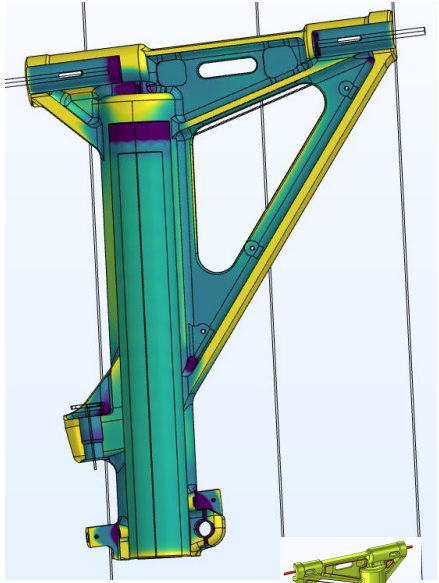
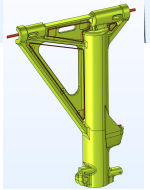
# MULTIPHYSICS AND MULTISCALE MODELING OF SURFACE FINISHING PROCESSES

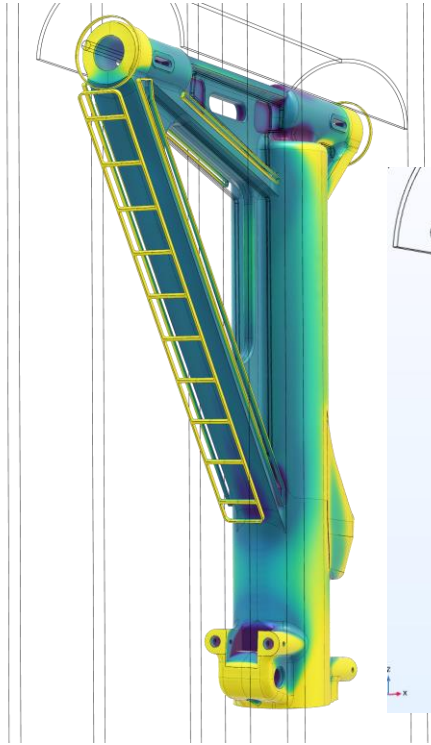
- Auxiliary anodes can be used to improve thickness distribution, but edge effects are always present
- Using current robber and insulated mask allows to reduce thickness heterogeneity

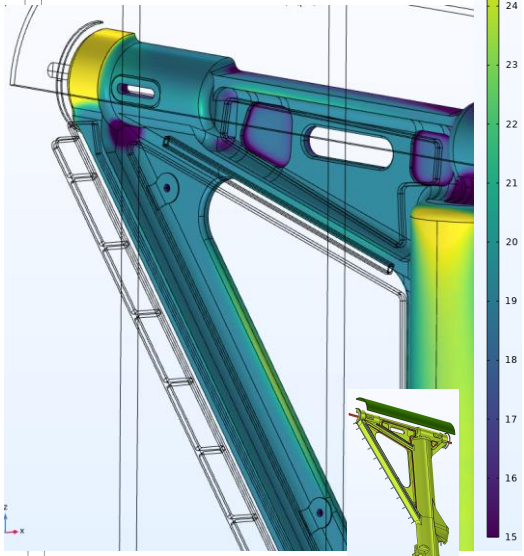


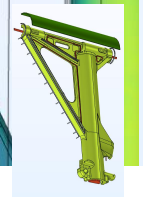


Thickness distribution (µm)









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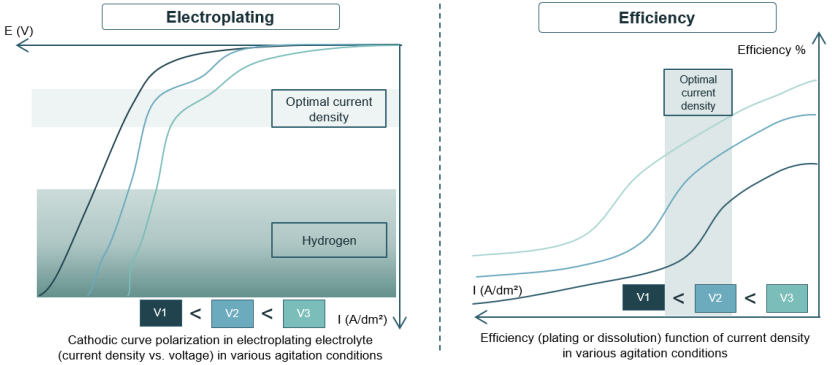
# MULTIPHYSICS AND MULTISCALE MODELING OF SURFACE FINISHING PROCESSES

- The geometric configuration of the electrochemical cell has a significant impact on thickness distribution, but this is not enough to anticipate all the mechanisms that could lead to thickness distribution problems or appearance defects
- Hydrodynamics can disrupt local electrochemical kinetics in two ways:
  - Depletion of active species
  - Accumulation of hydrogen in confined areas.

1 (Nernst-Planck) $\frac{\partial n_i}{\partial t} = \nabla \cdot [D_i \nabla n_i + \mu_i n_i \nabla \phi - n_i \mathbf{u}]$ (diffusion, migration, convection)

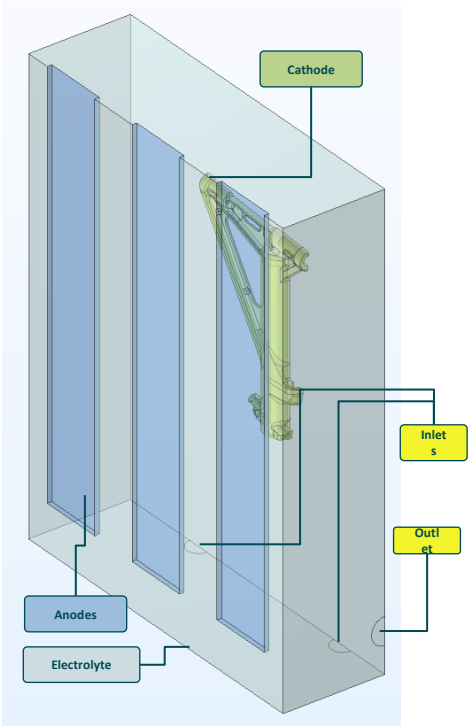
$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) = -\nabla p + \eta \nabla^2 \mathbf{u} - \nabla \phi \sum_{i=1}^{N} z_i e n_i$ (Navier-Stokes) $\nabla \cdot \mathbf{u} = 0$

$\nabla^2 \phi = -\frac{1}{\epsilon \epsilon_0} \sum_{i=1}^{N} z_i e n_i$ (Poisson)




Cathodic curve polarization in electroplating electrolyte (current density vs. voltage) in various agitation conditions

Efficiency (plating or dissolution) function of current density in various agitation conditions




CFD simulation in order to identify areas of low local fluid agitation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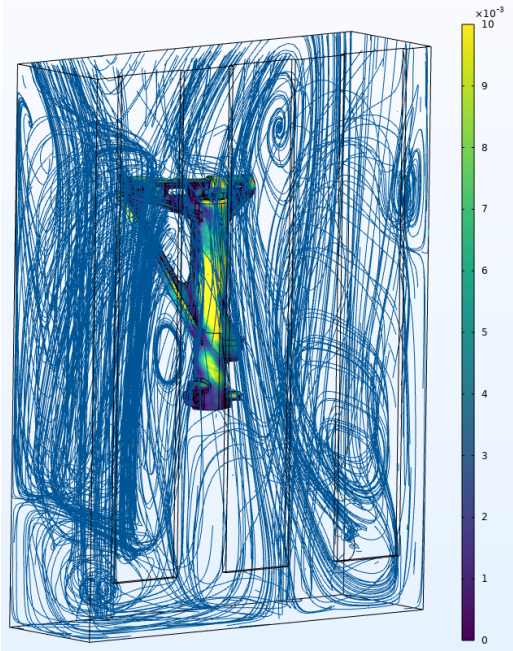
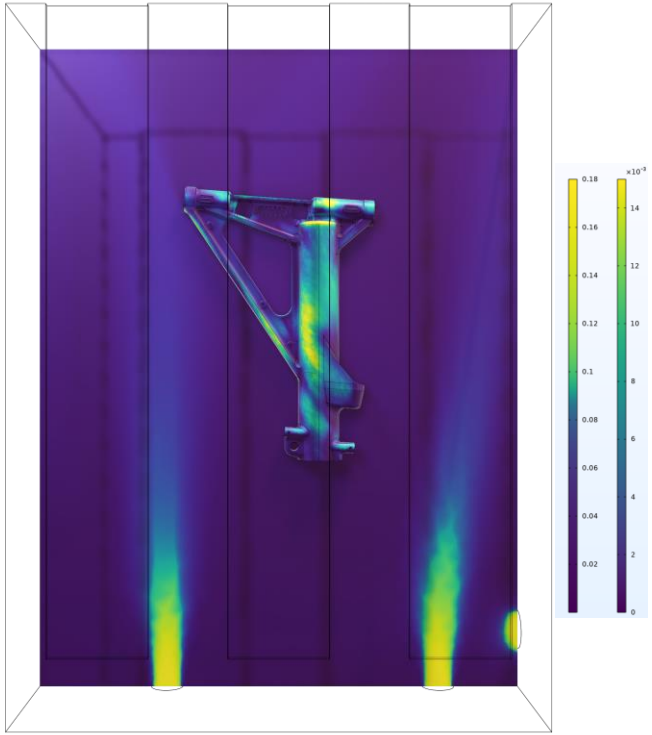
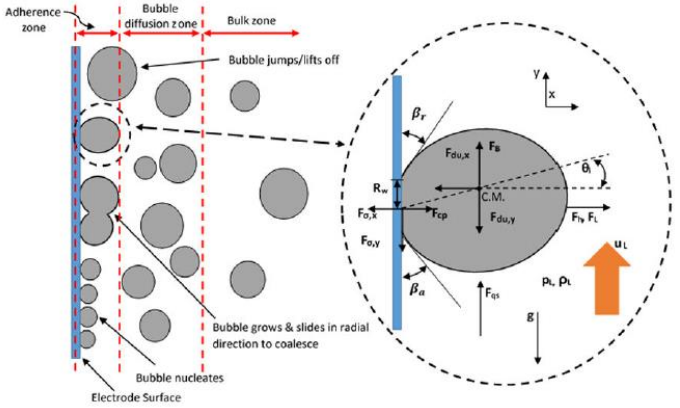
# MULTIPHYSICS AND MULTISCALE MODELING OF SURFACE FINISHING PROCESSES

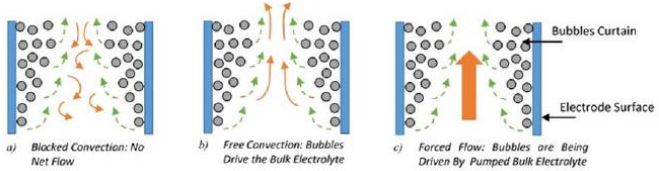
- Monophasic CFD modeling at the industrial scale using SST turbulent model
- Low agitation in internal pipes
- There is a deficiency in terms of penetration of the electric field lines, but also in terms of renewal of the active species




Flow speed (m/s)




J Electrochem Soc. 2017 ; 164(13): E448–E459. doi:10.1149/2.1161713jes.

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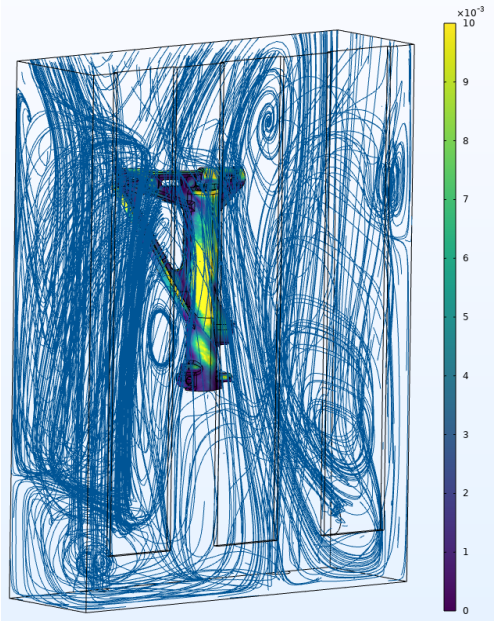


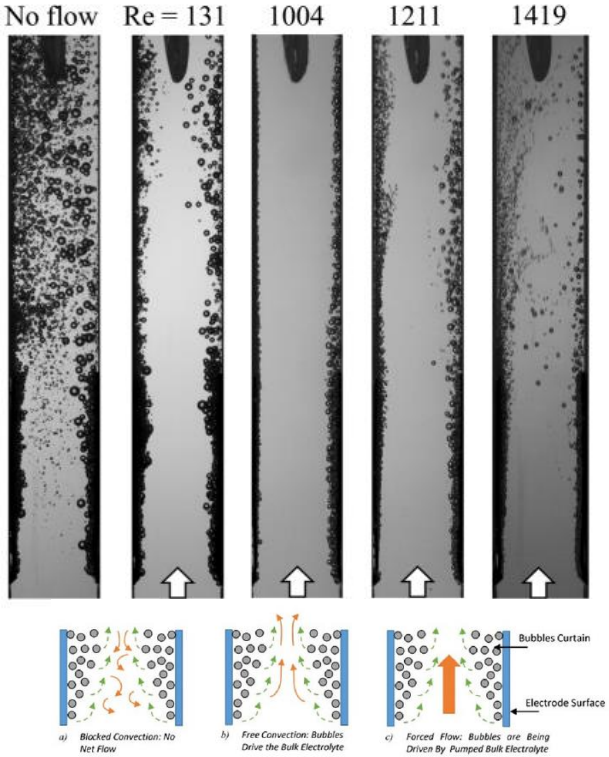


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Needs to design local agitation to improve species renewability and hydrogen elimination

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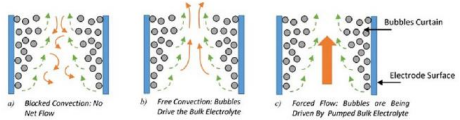
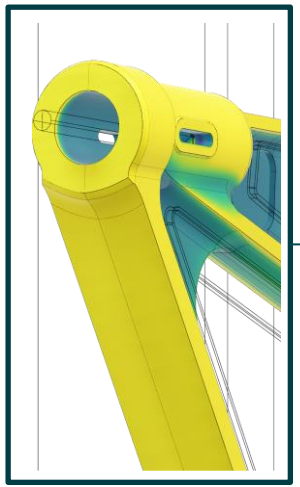
# MULTIPHYSICS AND MULTISCALE MODELING OF SURFACE FINISHING PROCESSES

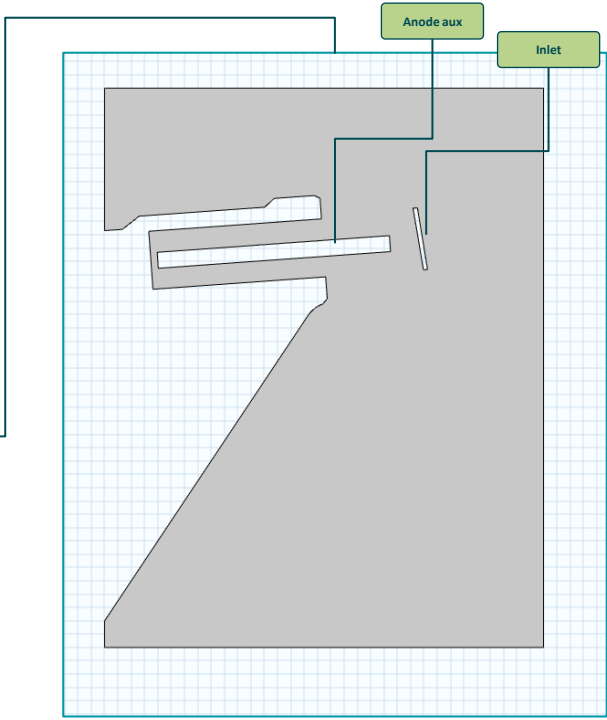
- In order to model all the involved phenomena within manageable computation times, we decided to switch to 2D cross-section
  - Additionally, the tertiary current distribution was coupled with bubbly flow

- This multiphysics approach investigate the reciprocal effect between electrodeposition, hydrogen evolution and electrolyte flow
  - Hydrogen bubbles are generated according to local current density and efficiency

  → Study of the impact of localized recirculation nozzle on hydrogen accumulating in the channel
- It is important to predict the evolution of hydrogen bubbles
  - Hydrogen production is a parasitic reaction
  - Hydrogen accumulation on the surface can create defect in coating







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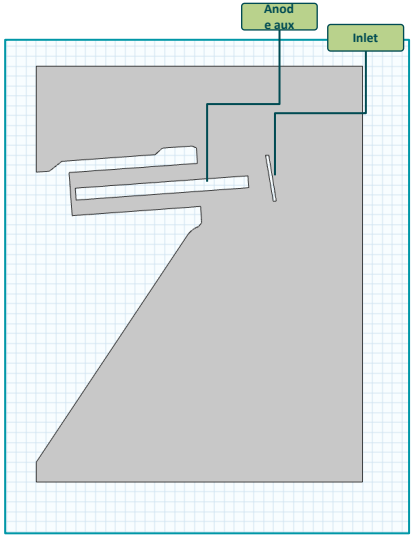
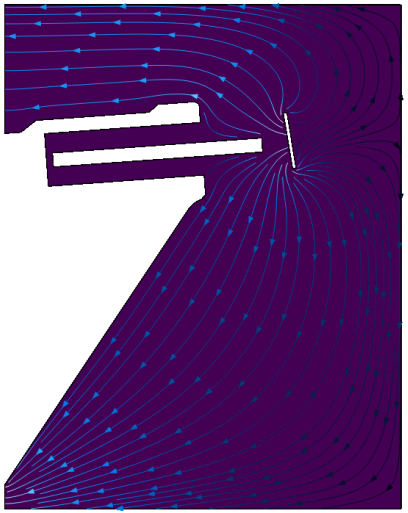
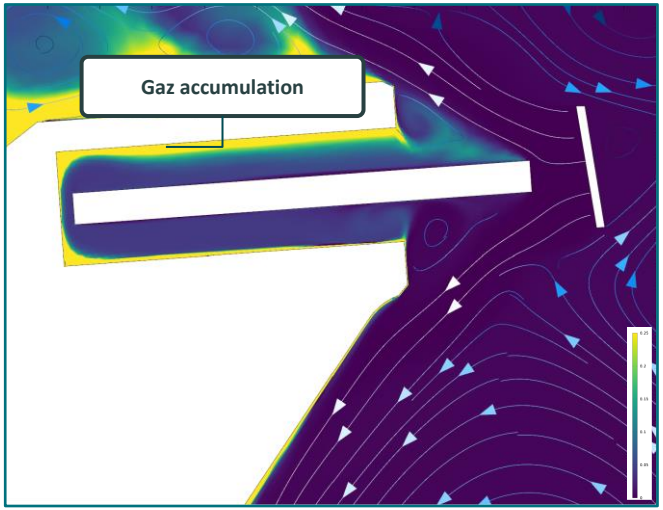
# MULTIPHYSICS AND MULTISCALE MODELING OF SURFACE FINISHING PROCESSES

- Tertiary current distribution coupled with Laminar bubbly flow, with hypothesis :
  - Hydrogen production is a function of local efficiency
  - Spherical bubble, diameter = 50 µm
  - Drag coefficient model : Hadamard–Rybczynski



Volumic gas fraction




Volumic gas fraction

- Hydrodynamics conditions needs to be optimized to avoid defects on surface and coating due to hydrogen generation and accumulation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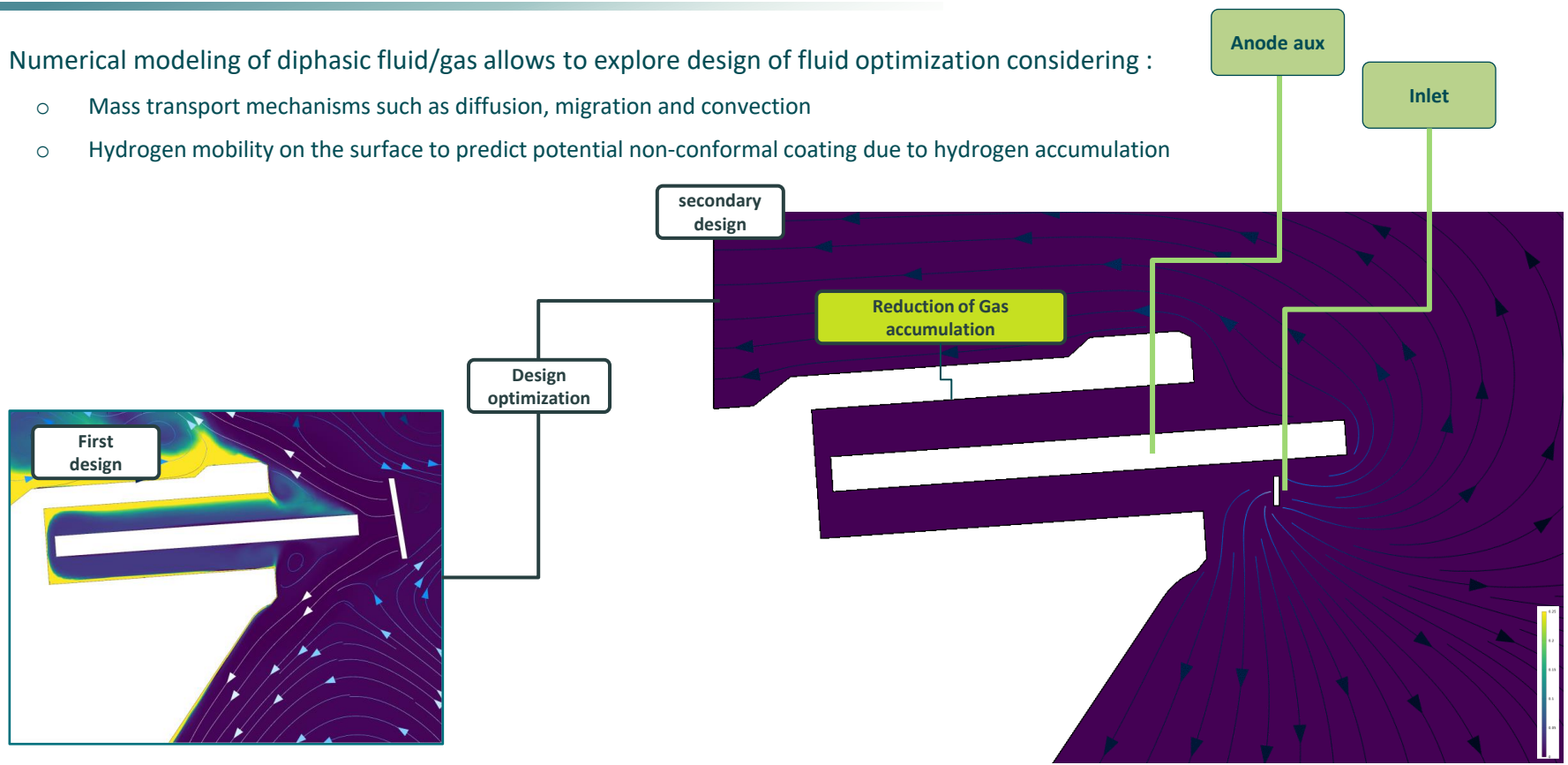
# MULTIPHYSICS AND MULTISCALE MODELING OF SURFACE FINISHING PROCESSES

- Numerical modeling of diphasic fluid/gas allows to explore design of fluid optimization considering :
  - Mass transport mechanisms such as diffusion, migration and convection
  - Hydrogen mobility on the surface to predict potential non-conformal coating due to hydrogen accumulation




Volumic gas fraction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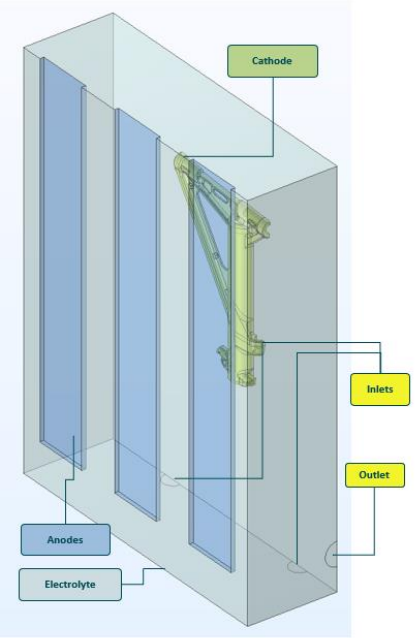
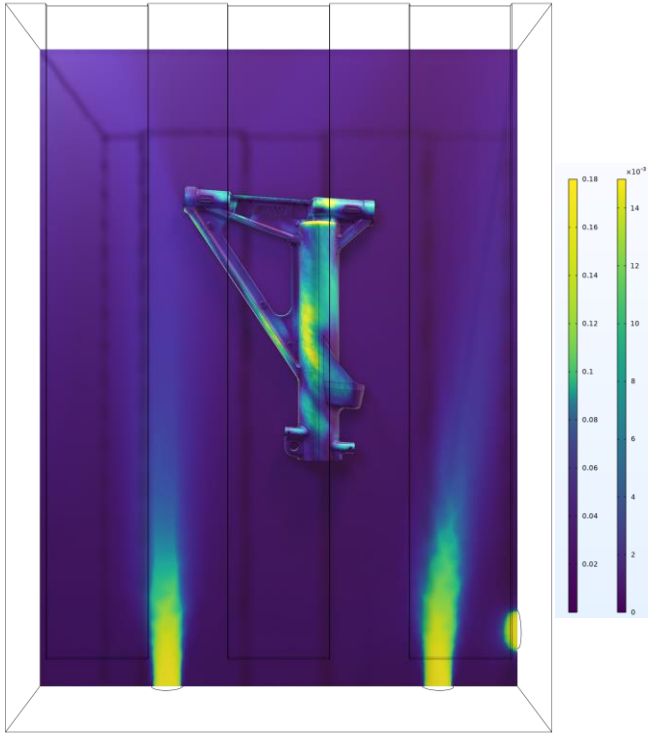
# MULTIPHYSICS AND MULTISCALE MODELING OF SURFACE FINISHING PROCESSES

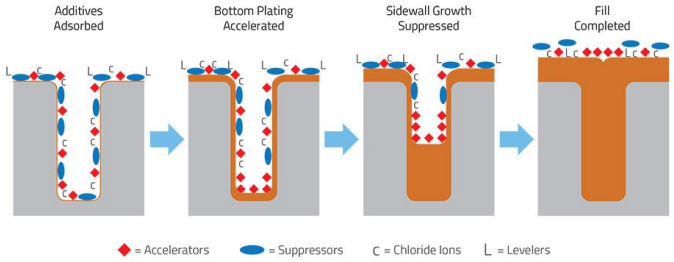
- Monophasic CFD modeling at the industrial scale using SST turbulent model
- Low agitation in internal pipes
- There is a deficiency in terms of penetration of the electric field lines, but also in terms of renewal of the active species




Flow speed (m/s)

Needs to design local agitation to **improve species renewability** and hydrogen elimination




J Electrochem Soc. 2017 ; 164(13): E448–E459. doi:10.1149/2.1161713jes.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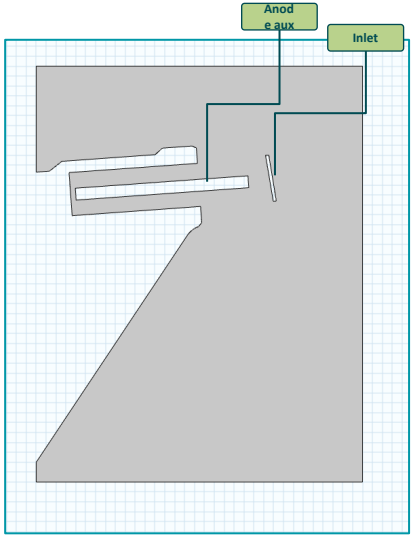
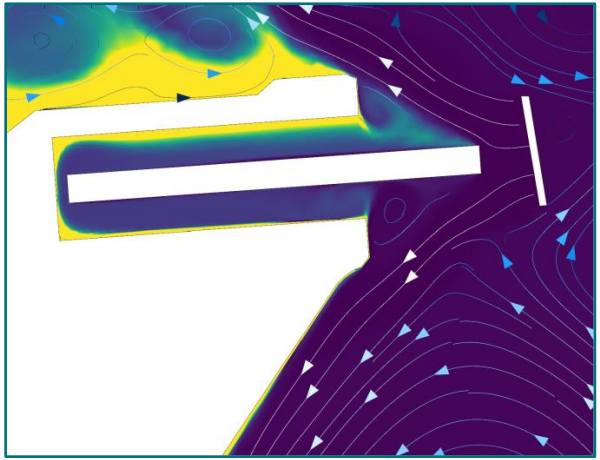
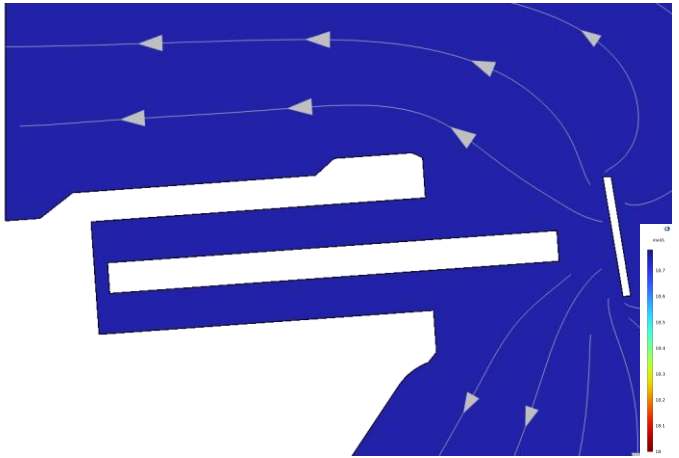
# MULTIPHYSICS AND MULTISCALE MODELING OF SURFACE FINISHING PROCESSES

- Tertiary current distribution allows to introduce mass transport of additive :
  - Mass transport of additives due to convection
  - Additive consumption coupled with electrochemical kinetics
  - Efficiency depends on local current density and additive concentration



Volumic gas fraction



Additive concentration

- Additive concentration decreases due to electrochemical reaction
- If local hydrodynamic conditions are not sufficient to replenish additive concentration

→ impact coating properties (thickness, microstructure, …)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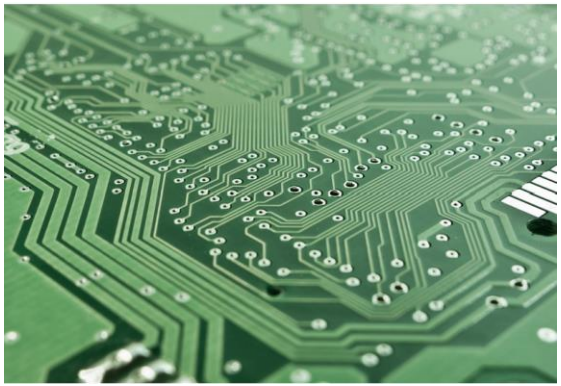
# MODELING EXPLICIT COATING GROWTH AT LOCAL SCALE

- Explicit modeling of coating growth
- Anticipate defect du to local heterogeneous growth
- Useful for microelectronic application



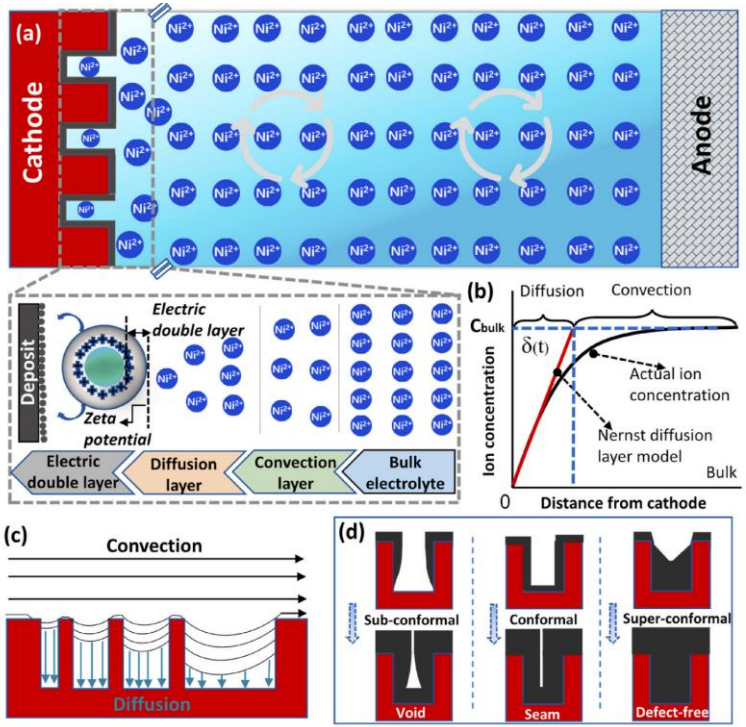



**Fig. 1.** Schematic of ion transportation and microstructural filling mechanisms during the electroforming process: (a) ion transportation in electrodeposition process; (b) diffusion theory; (c) convection-diffusion- dominated mass transfer; (d) different microstructural filling modes.

Zhang et al.https://doi.org/10.1016/j.precisioneng.2021.04.008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# MODELING EXPLICIT COATING GROWTH AT LOCAL SCALE

- ❑ Explicit modeling of coating growth
- ❑ Anticipate defect du to local heterogeneous growth
- ❑ Useful for microelectronic application

→ Moving Boundaries or level set

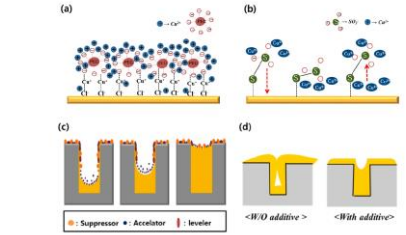
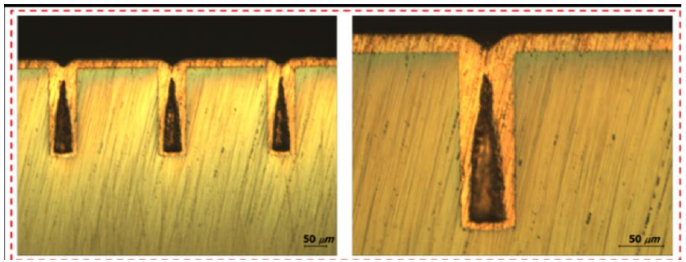
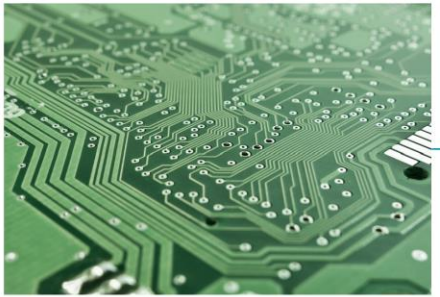
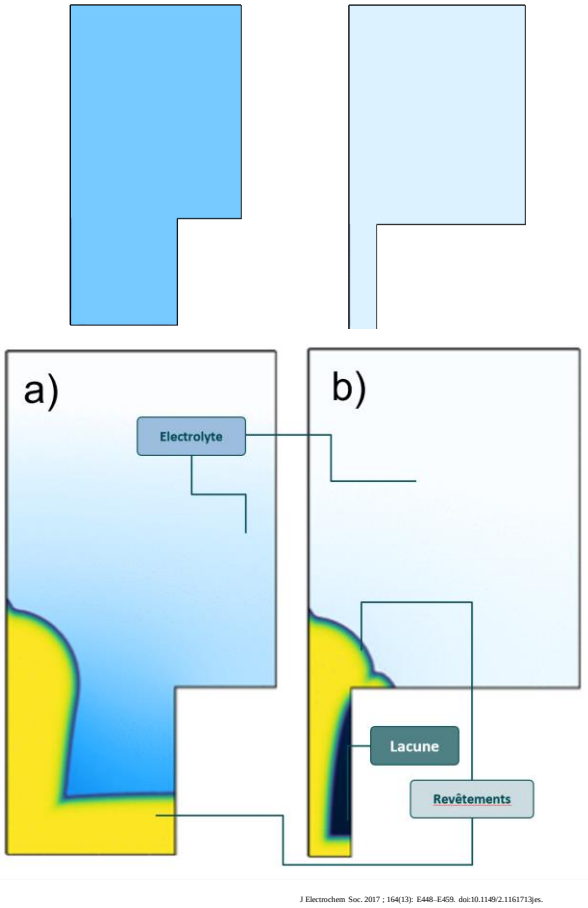



**Figure 5.** A schematic diagram of additive behavior in plating solution. Action of Cl ion: (**a**) PEG and (**b**) SPS in plating bath; (**c**,**d**) effect of additive in electrodeposition.




*Appl. Sci.* **2018**, *8*, 2135; doi:10.3390/app8112135



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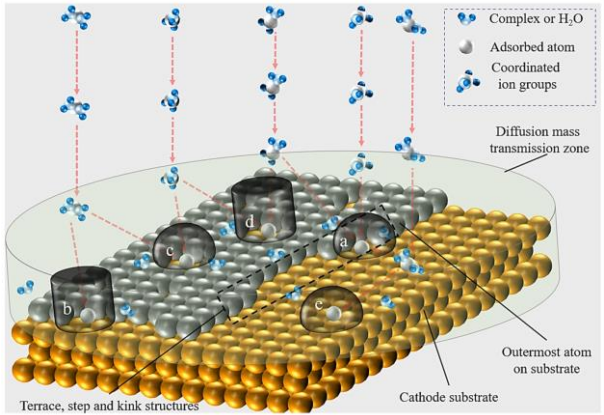
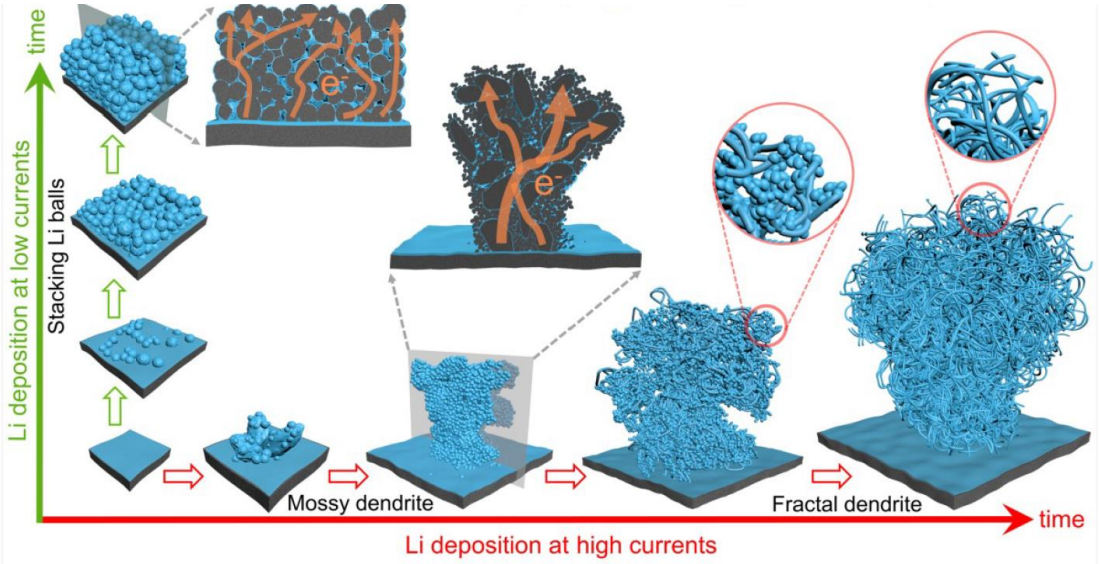
# ELECTROLYTIC COATING NUCLEATION

- Understanding of the initial stages of electroplated coating formation
- Can helps to anticipate where and how defects may form due to non-uniform growth rates
- Can helps to anticipate grain size and texture of the coating
- Homogeneous nucleation tends to produce a more uniform microstructure, while heterogeneous nucleation can lead to variability in grain sizes and distribution
- The nature of the electrolytic solution, applied current density, temperature, and other electroplating parameters can affect the type and distribution of nucleation → Influence final microstructure




Luo, G.; Yuan, Y.; Li, D.-Y.;Li, N.; Yuan, G.-H. Current Transition of Nucleation and Growth under Diffusion-Controlled Electrocrystallization: A Brief Review.Coatings **2022**, 12, 1195. https://doi.org/10.3390/coatings12081195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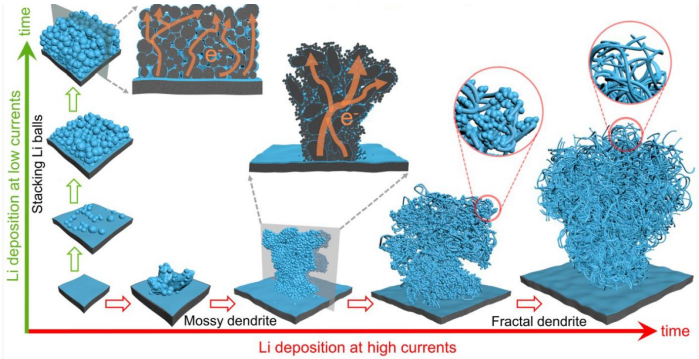


***Morphology and structure transition at varying deposition rates***

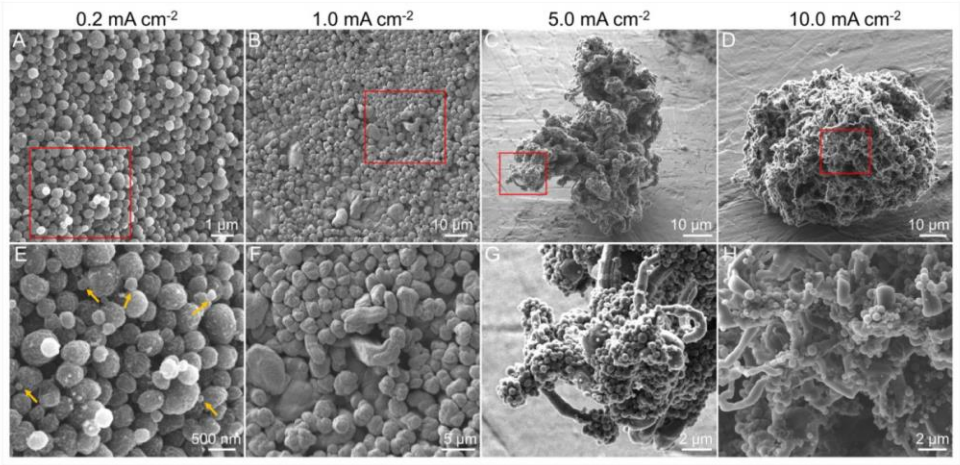


**Figure 1. Li morphology transformation with increasing deposition current.** (A-D) SEM images showing morphological features of Li deposition on Li substrates at current densities of 0.2, 1.0, 5.0, 10.0 mA $cm^{-2}$ for a fixed capacity of 1.0 mAh $cm^{-2}$; (E-H) Corresponding magnified images of the red squared regions in (A-D), respectively.

Luo, G.; Yuan, Y.; Li, D.-Y.;Li, N.; Yuan, G.-H. Current Transition of Nucleation and Growth under Diffusion-Controlled Electrocrystallization: A Brief Review.Coatings **2022**, 12, 1195. https://doi.org/10.3390/coatings12081195


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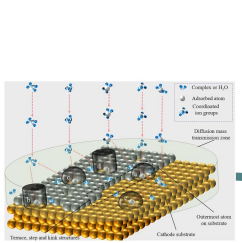
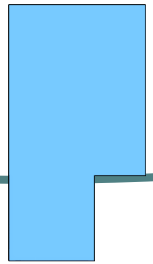
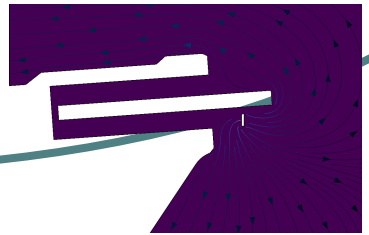
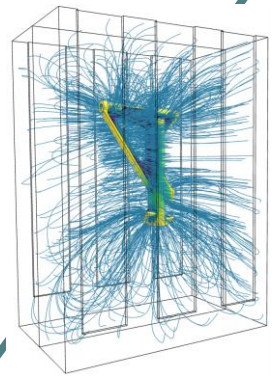
# INTERMEDIATE CONCLUSION

- **Multiphysics and multiscale modeling of electroplating processes allows to :**
  - Improve fundamental process understanding
  - Optimize and reduce treatment heterogeneity and non-quality
  - Reduce wasted material
  - Reduce time and cost for electroplating tooling development by virtual prototyping
  - Help to define best practice in industrial surface finishing processes
  - Innovate and explore alternative production methods
  - Increase reactivity to implement new coating (Reach) or finishing new geometries (AM parts)







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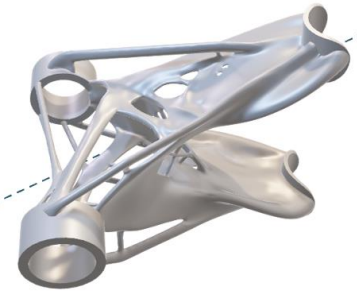
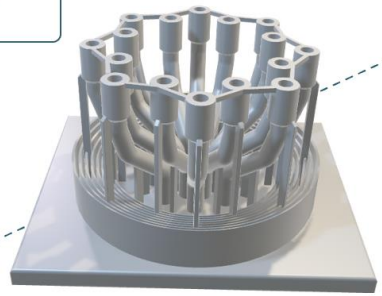
# ADDITIVE MANUFACTURING : BENEFITS AND DRAWBACKS

**Benefits**

- Lightweighting
  - Optimize part structure
  - Lower material consumption
  - Add / combine functionalities
- Graded materials
  - Fast prototyping
  - Assembly part reduction
  - Organic geometry
- Innovation
  - Less waste





**Drawbacks**

- Surface finishing
  - Unmelted powder
  - Roughness
  - High shape factor and small details
- Complex geometry
  - Non conventional geometry

→ *Additive manufacturing parts need to be finished to improve surface properties*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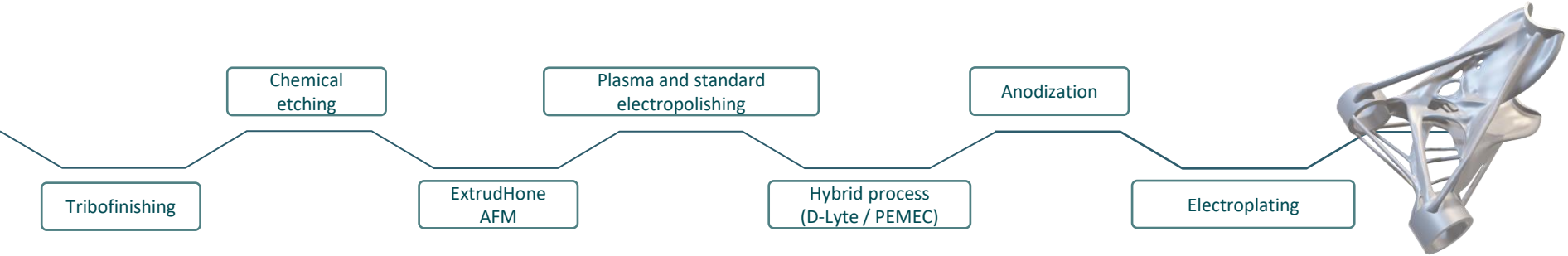
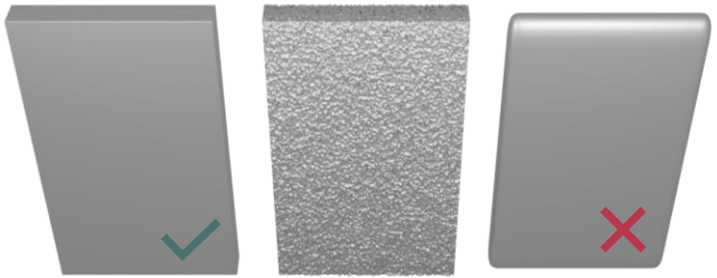
# SURFACE FINISHING OF ADDITIVE MANUFACTURING PART

- Several processes are investigated to improve the surface finish of additive manufacturing parts by adding or removing material.




- New and hybrid surface finishing processes and well-known surface finishing processes need to be adapted to meet the challenges of AM parts
- AM parts also need coatings (anodization, electroplating...) for functional and aesthetic properties

→ Accessibility on complex geometry parts



**→ The challenge is to be able to control these processes optimally in order to obtain the good surface roughness while at the same time minimizing shape distortion**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# SURFACE FINISHING OF ADDITIVE MANUFACTURING PART

**Risk of failure to achieve post processing conformity**

**Internal network**
**Complex shape / High shape factor**

**Fluid accessibility** and fluid flow

**Products removal** (unmelted powder, oxide…)

**Gas retention** during chemical and electrochemical processes

**Local current distribution** during electrochemical processes

**Thin walls**

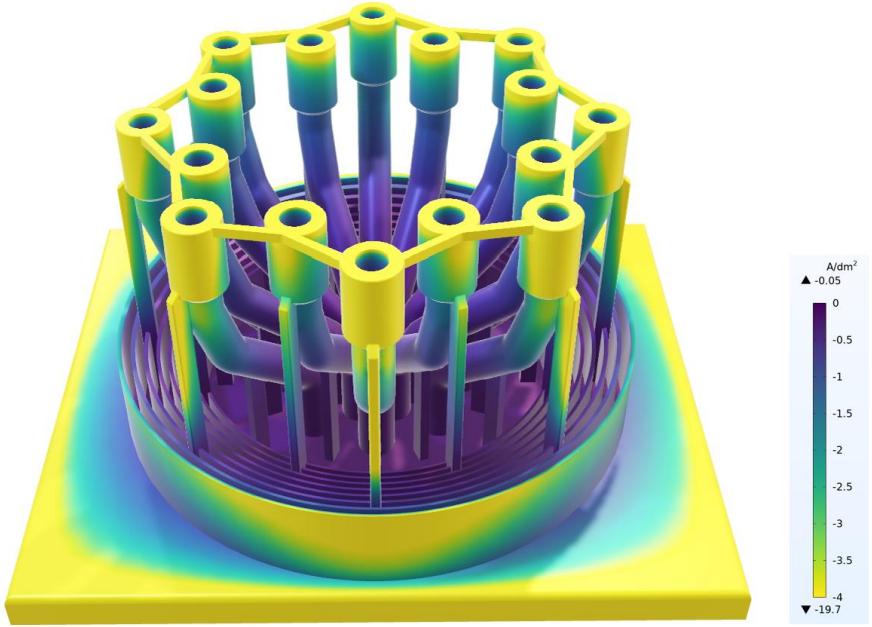
Hole formation
**Excessive attack**

**Sharp design**
**High shape ratio**

**Edge smoothing**

**Lack of coating**

**Current distribution without tooling**





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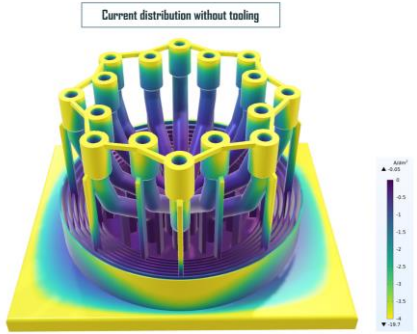


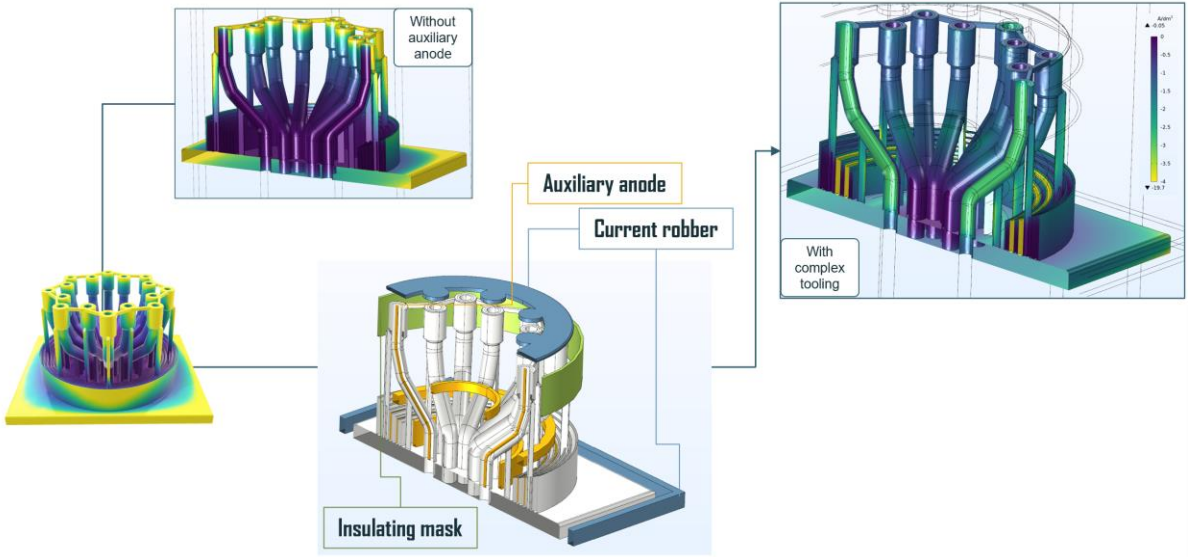



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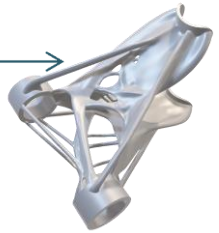
# SURFACE FINISHING OF ADDITIVE MANUFACTURING PART

Chemical etching → Plasma and standard electropolishing → Anodization

Tribofinishing → ExtrudHone AFM → **Hybrid process (D-Lyte / PEMEC)** → Electroplating



Particules électrochimiquement actives (résines échangeuses d'ions)
Electrolyte support non oxydant

Source : https://www.gpainnova.com/

Particules électrochimiquement inactives (media de tribofinition)
+ Electrolyte d'électropolissage

CENTRALELYON ENISE — cetim — INSTITUT CARNOT Ingénierie@Lyon

Polissage Electro-Mécano-Chimique
PEMEC

Source : https://www.ingenierie-at-lyon.org/projet/2020-pemec-pollisage-electro-mecano-chimique/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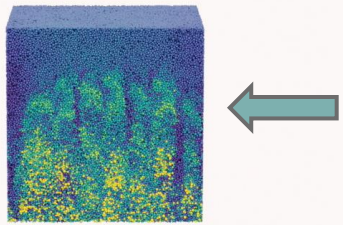
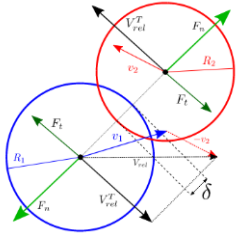
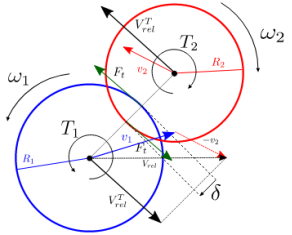
# HOW TO MANAGE THE SPECIFIC SIMULATION LINKED TO HYBRID PROCESSES

- **Granular modeling at the process scale → Discrete element method optimized on GPU**
  - Simulation of particle kinematics and interaction with the surface to be treated
  - Prediction of particle/particle and particle/workpiece interactions (contact force, contact time, number of contacts, speed, acceleration, etc.)

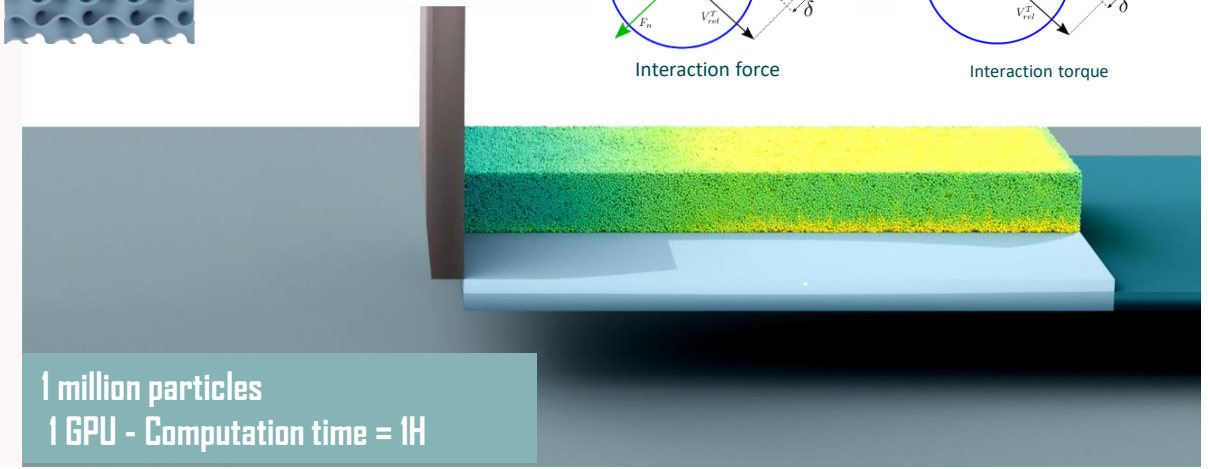


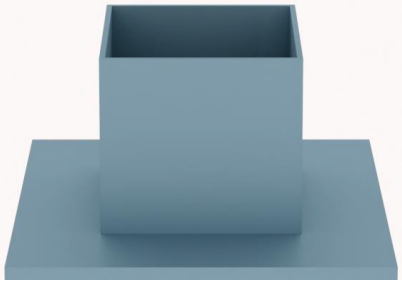


Interaction force



Interaction torque

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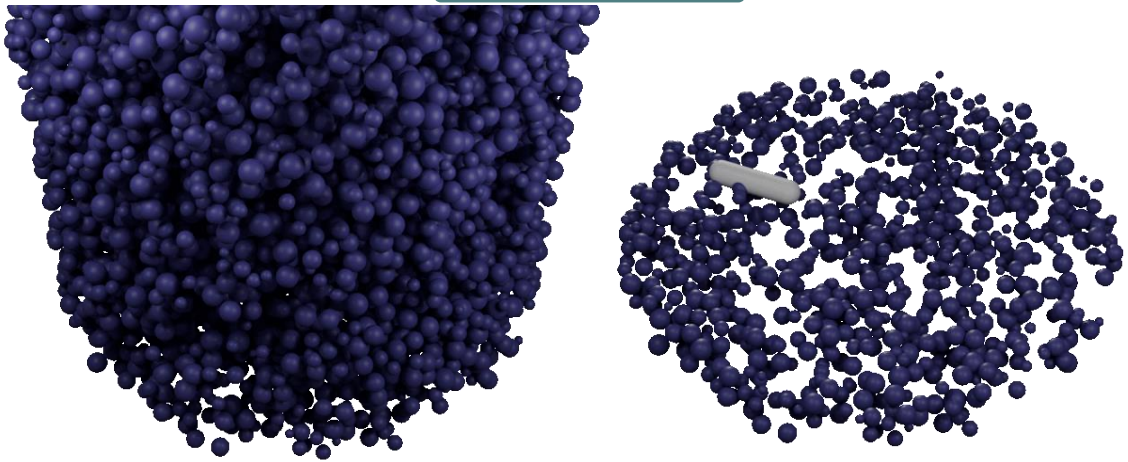
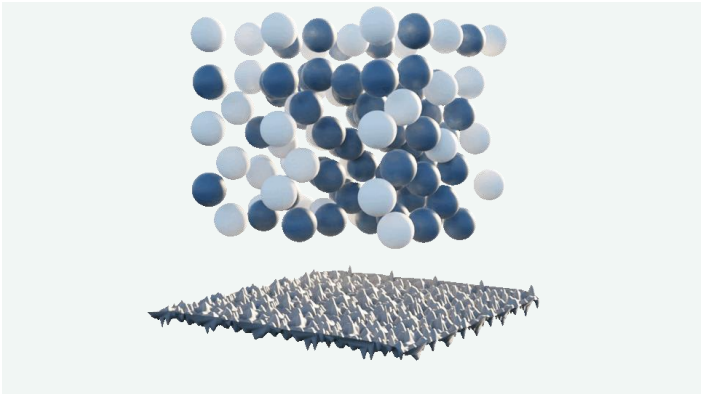
# HOW TO MANAGE THE SPECIFIC SIMULATION LINKED TO HYBRID PROCESSES

- **Granular modeling at the process scale → Discrete element method optimized on GPU**
  - Simulation of particle kinematics and interaction with the surface to be treated
  - Prediction of particle/particle and particle/workpiece interactions (contact force, contact time, number of contacts, speed, acceleration, etc.)

MACRO SCALE



MICRO SCALE

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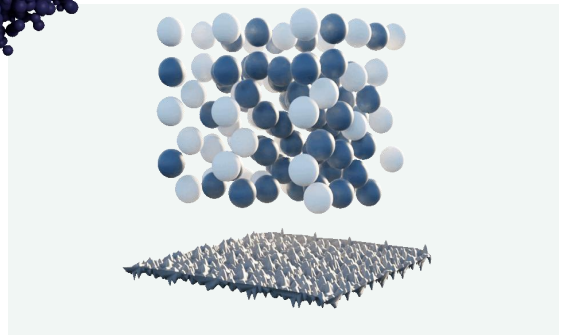
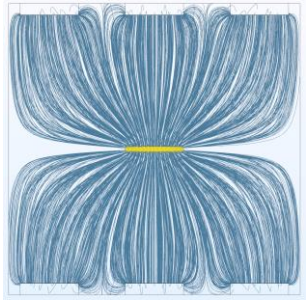
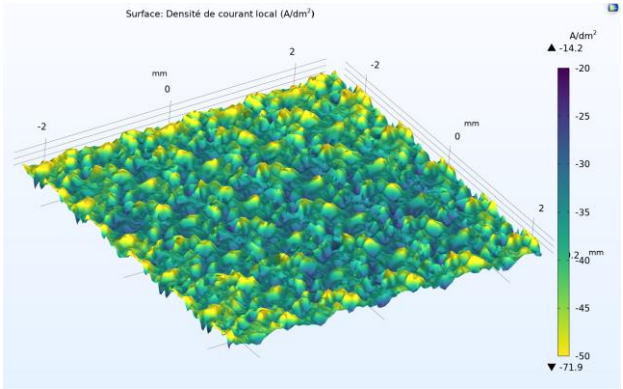
# HOW TO MANAGE THE SPECIFIC SIMULATION LINKED TO HYBRID PROCESSES

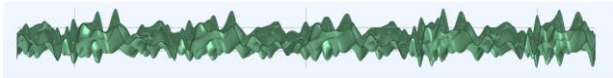
- Granular modeling gives information about particle/surface interactions
- Inputs for finite element modeling of electrochemical phenomena at macro and local scale





Modeling local current density at roughness scale

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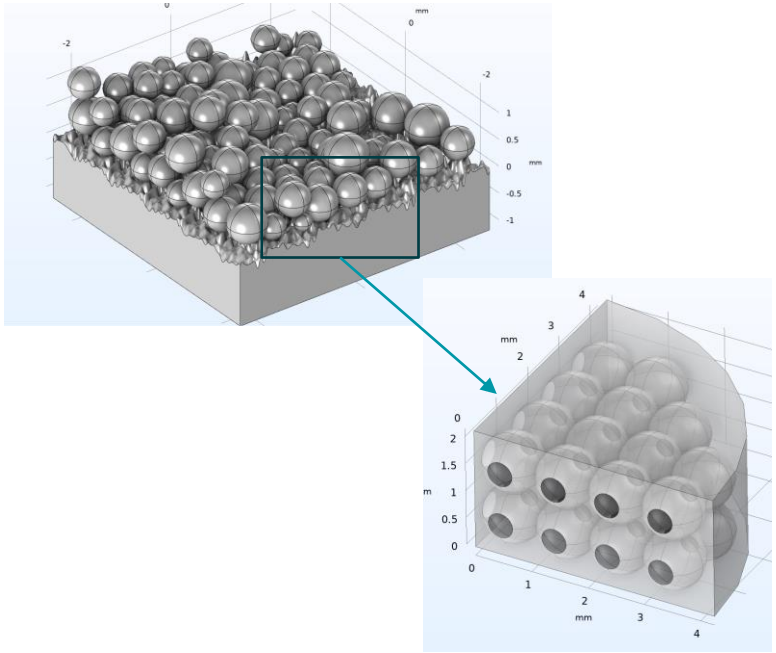
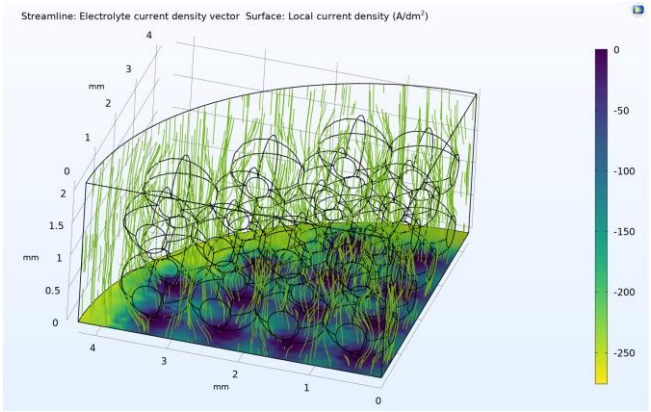
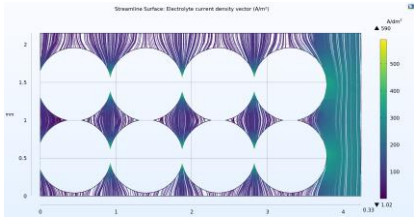
# HOW TO MANAGE THE SPECIFIC SIMULATION LINKED TO HYBRID PROCESSES

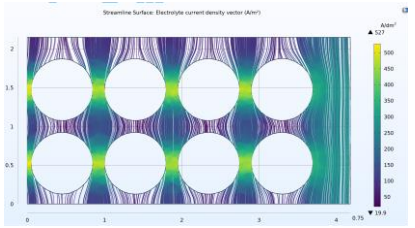
- **Needs to develop link between DEM and FEM**
  - Input particles distributions in FEM
  - Particles modify current line distribution

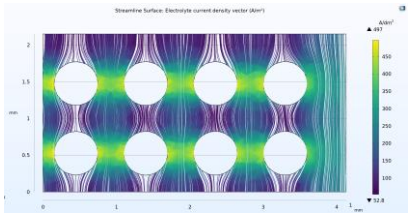
PEMEC







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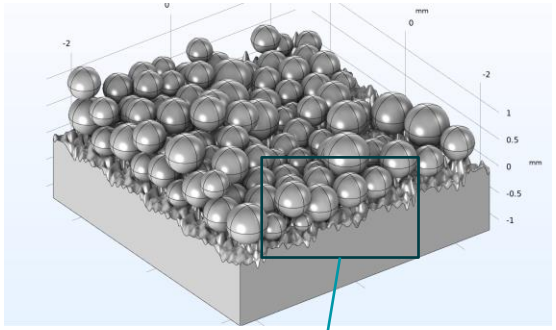
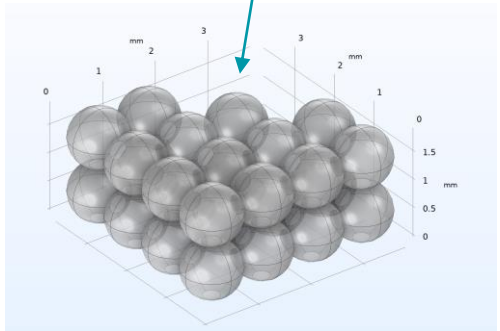
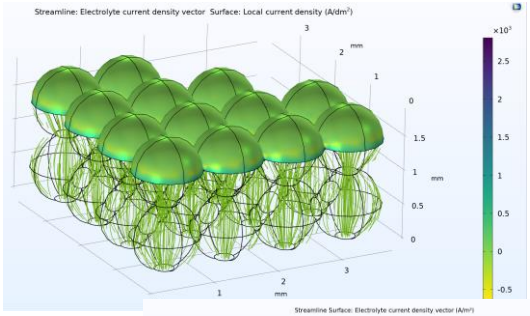
# HOW TO MANAGE THE SPECIFIC SIMULATION LINKED TO HYBRID PROCESSES

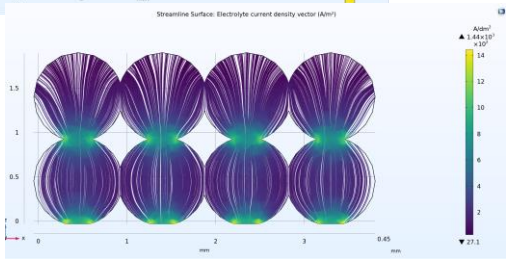
- **Needs to develop link between DEM and FEM**
  - Input particles distributions in FEM
  - Particles conduct current in porous media





DLyte




Link with transport through porous media (Battery application)

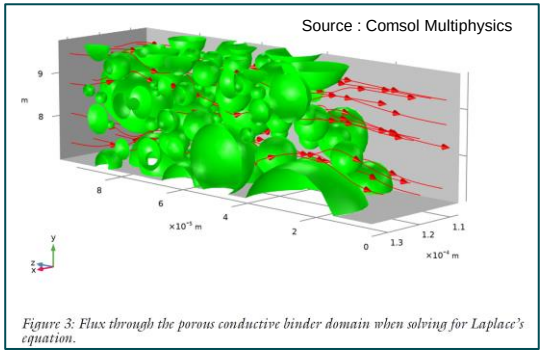
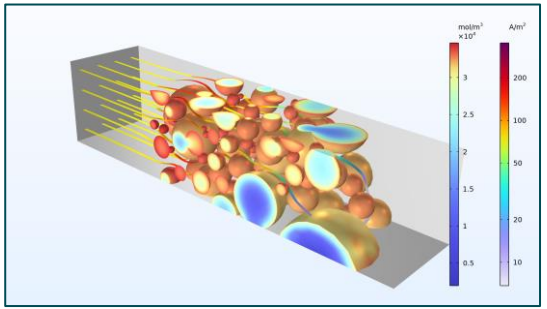



*Figure 3: Flux through the porous conductive binder domain when solving for Laplace's equation.*

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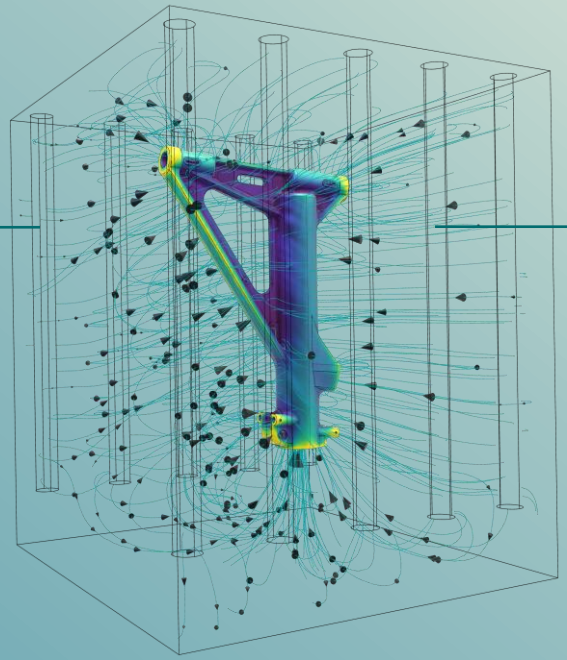
# HYBRID PHYSIC-BASED / DATA DRIVEN MODELING

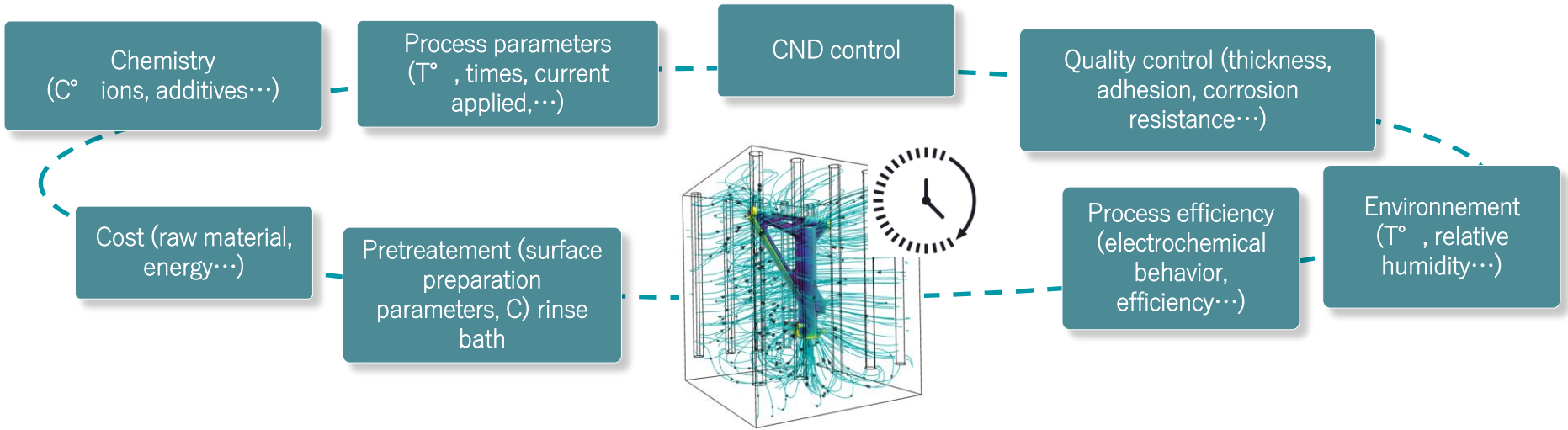
MULTIPHYSICS MODELING



DATA SCIENCE AND IA

# DATA SCIENCE APPLIED TO SURFACE TREATMENT

**An industrial workshop of surface treatment is essentially a vast active database of useful information**




**It is essential to break the boundaries between data to encourage interaction and collaboration between the different profession**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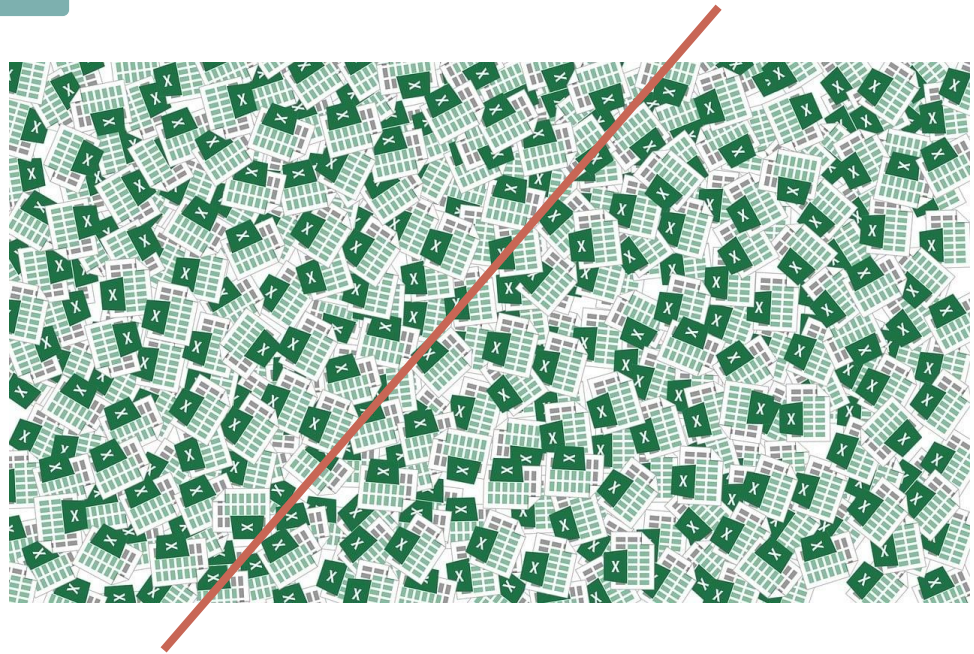
# DATA SCIENCE APPLIED TO SURFACE TREATMENT

**DATA**

- Define problem / goal
- Raw data collection
- Data cleansing and validation

Exploratory Data Analysis

Make decision





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# DATA SCIENCE APPLIED TO SURFACE TREATMENT

**DATA**

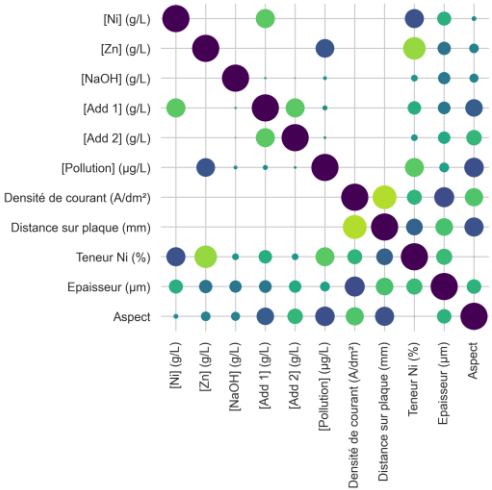
- Define problem / goal
- Raw data collection
- Data cleansing and validation

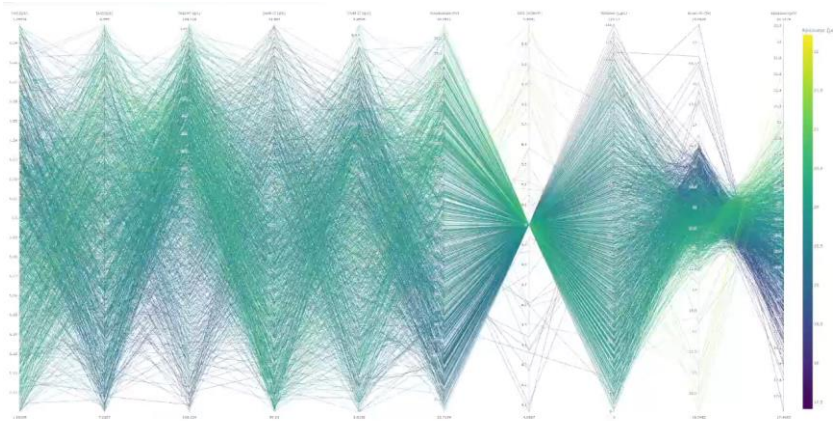
Exploratory Data Analysis

Process parameters (current, electrode distance)

Chemistry (C° ions, additives, pollution…)

Make decision

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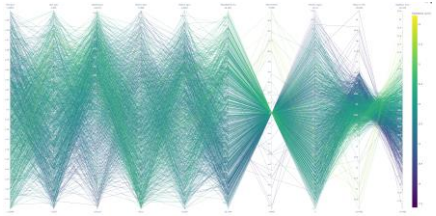
# DATA SCIENCE : ML DECISION SUPPORT TOOLS

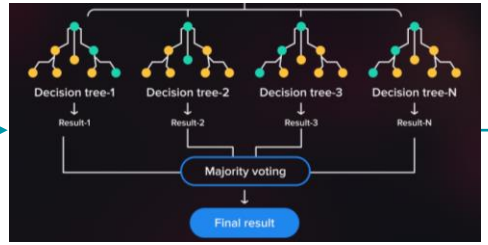
**DATA**

- Define problem / goal
- Raw data collection
- Data cleansing and validation

Exploratory Data Analysis

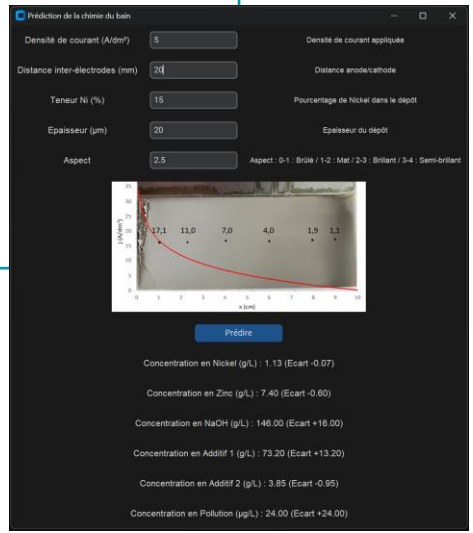


Machine learning modeling




https://serokell.io/blog/random-forest-classification

Make decision




- A decision-making support tool that capitalizes on experience via ML algorithms
- Reverse problem solving / Output results --> Input parameters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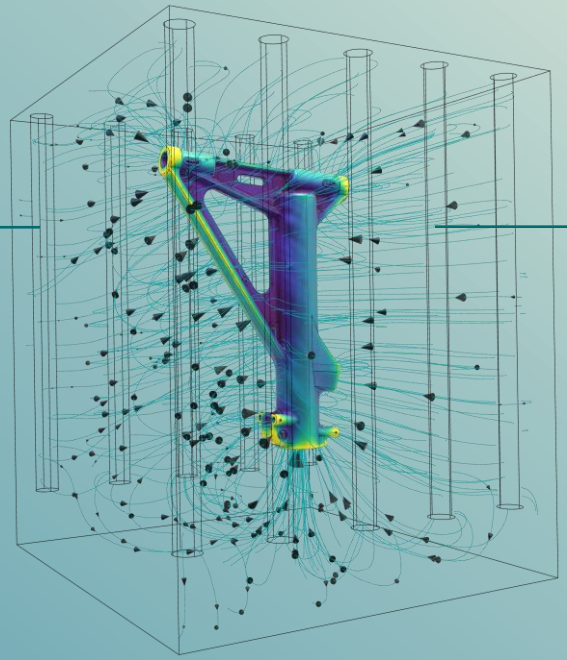
# HYBRID PHYSIC-BASED / DATA DRIVEN MODELING

## MULTIPHYSICS MODELING

- **Physics based** models are **powerful**, **robust** and can be **predictive**
- Predictivity is possible from a **small amount of data**
- Prediction accuracy depends on initial assumptions
- Requires repeating characterizations when chemistry modifications occur
- Multiphysics and high-fidelity modeling can improve prediction performance, but it can get **complex** and **expensive**
- In industrial environments, surface finishing processes involve a temporal evolution of multiple parameters (additive concentration, conductivity, pollution...) which must imperatively be considered



## DATA SCIENCE AND IA

- **Data driven** modeling allows identification of **links** and **patterns** between an infinity of parameters → **predictive relationship between inputs and outputs**
- But requires **a lot of data** to be predictive
- But requires careful work regarding the data to be studied (identification, **cleaning**, classification..)
- Need to develop exploration and post-treatment tools of results in order to **extract value from data**
- Need an **expert** to identify data and evaluate trained models
- **A purely statistical approach** is complex to implement on special processes in an industrial environment → IA effectiveness (ML algorithm) depends on the representativeness and completeness of data

## Hybridization Physic-based - Data driven

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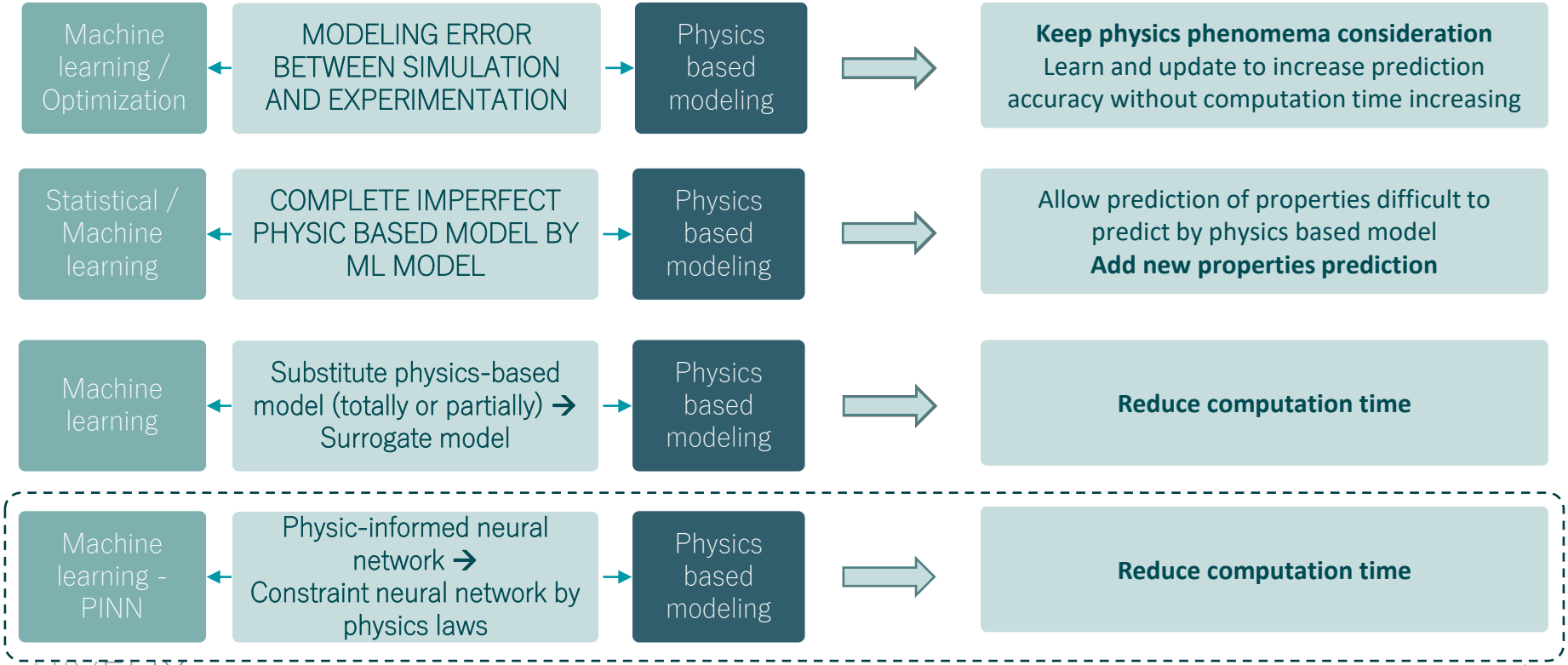
# HYBRID PHYSICS-BASED AND DATA-DRIVEN MODELING

❑ A **hybrid approach** is useful to take **advantages** of well-known methodologies of simulation (physics-based modeling) and new modeling tools link to data





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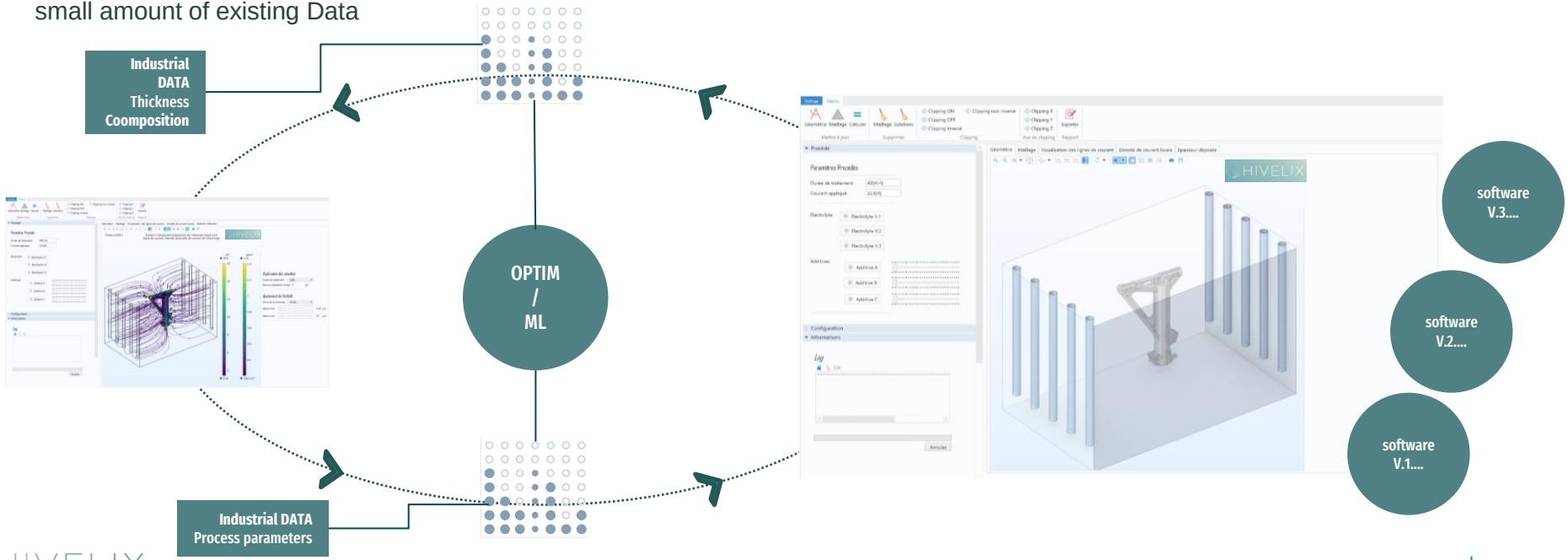
# HYBRID PHYSIC-BASED / DATA DRIVEN MODELING - Improve model accuracy

- Use of industrial data to improve predictions of physical models via error analysis
- Improve physic-based model with real industrial data, continuous learning and optimization
- Considering variability from industrial environments with a small amount of existing Data

Machine learning / Optimization ← MODELING ERROR BETWEEN SIMULATION AND EXPERIMENTATION → Physics based modeling





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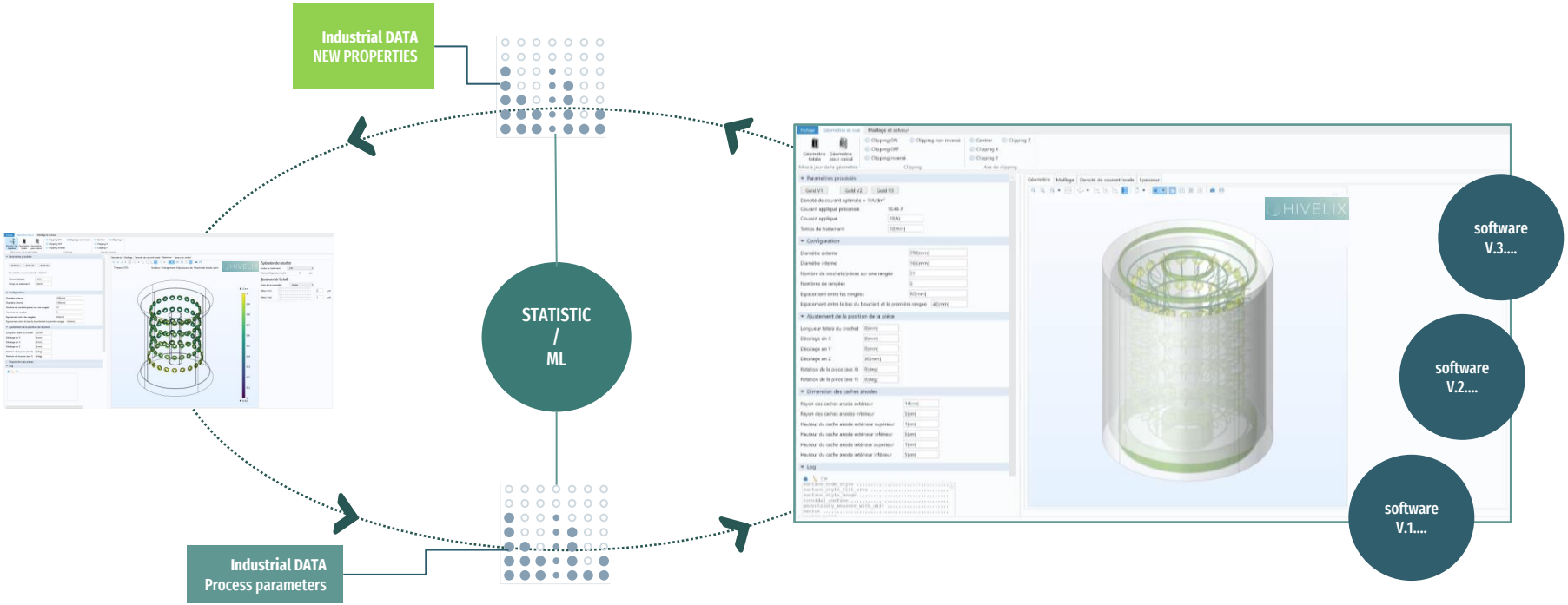
# HYBRID PHYSIC-BASED / DATA DRIVEN MODELING - Predict new properties

Statistical / Machine learning ← COMPLETE IMPERFECT PHYSIC BASED MODEL BY ML MODEL → Physics based modeling





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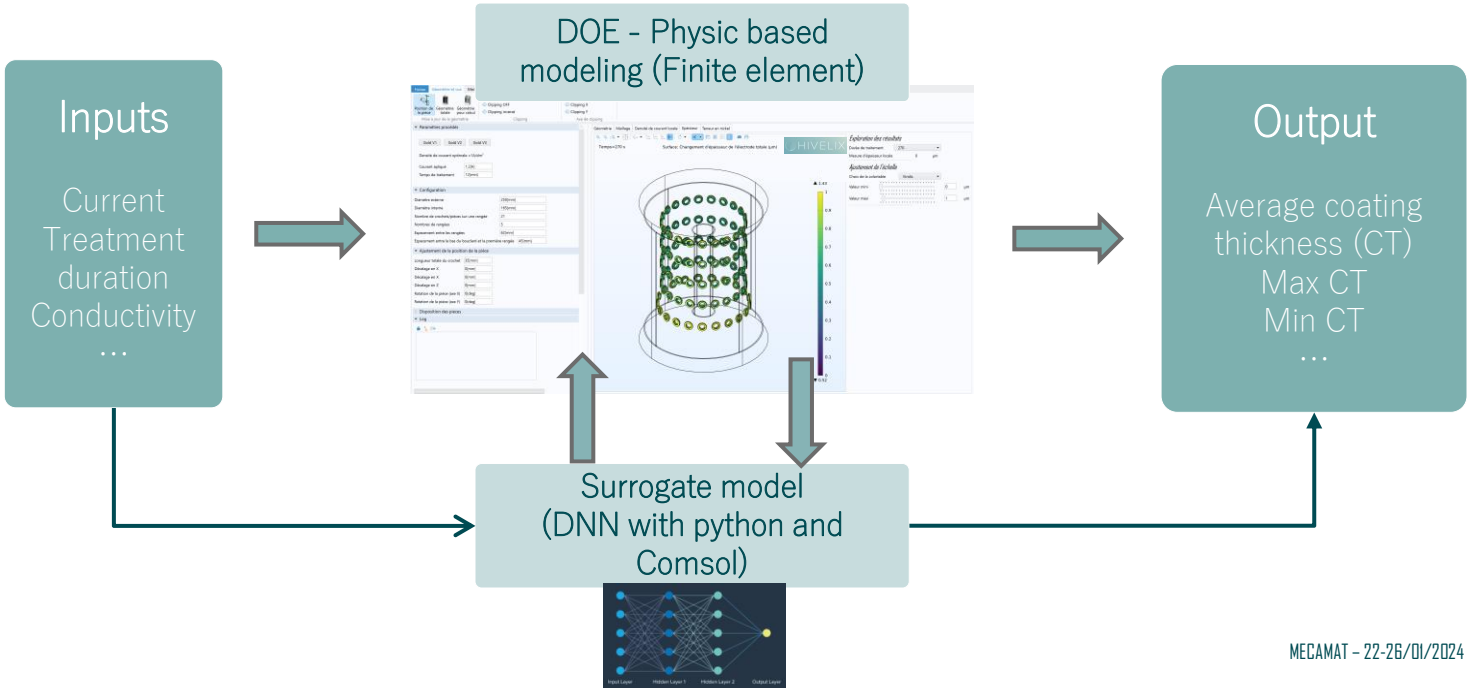
# HYBRID PHYSIC-BASED / DATA DRIVEN MODELING - Predict new properties

- Surrogate model advantages :
- Provides a computationally efficient approximation of complex physical models.
- Enables real-time or near-real-time predictions, essential for rapid decision-making.
- Ideal for process control and interactive simulations where fast computation is crucial.



# HYBRID PHYSIC-BASED / DATA DRIVEN MODELING - Physics-Informed Neural Networks

❑ **Physics-Informed Neural Networks (PINNs) :**

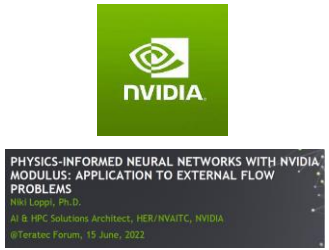
- Combine traditional data-driven machine learning with physics-based modeling.
- Incorporate known physical laws as prior information in the learning process.

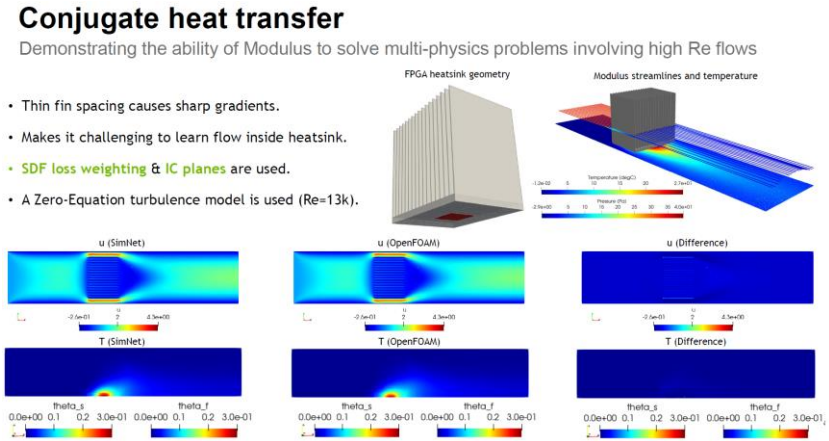
❑ **Advantages :**

- Enhanced prediction accuracy by integrating physical laws into neural network training.
- Reduction in required training data volume, as physics provides additional constraints.

❑ **NVIDIA MODULUS Library :**

- Enables the fusion of physical equations (PDEs) with data-driven approaches for robust model development.
- Designed for high performance with support for GPU-accelerated computing.
- Build high-fidelity, parameterized surrogate models with near-real-time latency.





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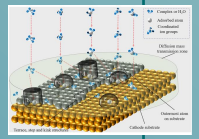
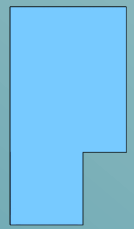
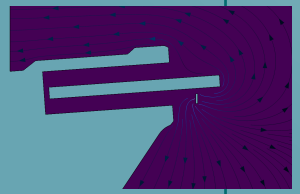
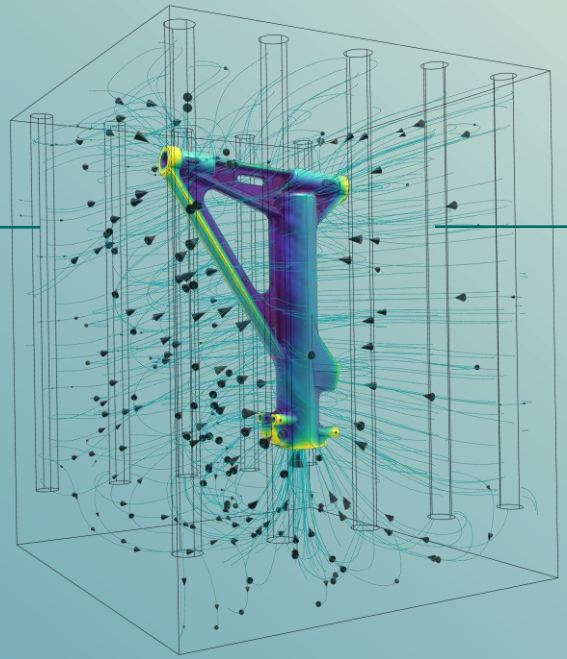
# SURFACE FINISHING OPTIMIZATION

MULTIPHYSICS MODELING

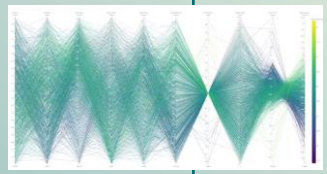








DATA SCIENCE AND IA



Hybrid modeling
Physic-based
-
Data driven

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# Thanks for your attention

**R&D** in multiphysics simulation

Custom **software** and **Digital Twin**

**Data Science / ML** applied to industrial processes

**Process optimisation** assisted by simulation

**Custom Training software** for education and industry

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COMSOL Certified Consultant