Using Artificial Intelligence (AI) within COMSOL Multiphysics® to Create Machine Learning Tools

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Outline

I. Background – Motivations – Objectives

II. Modelling and Numerical Model

III. Main Results

IV. Conclusions – Perspectives

***Before starting, who we are…* www.simtecsolution.fr**

SIMTEC : Fundamentals

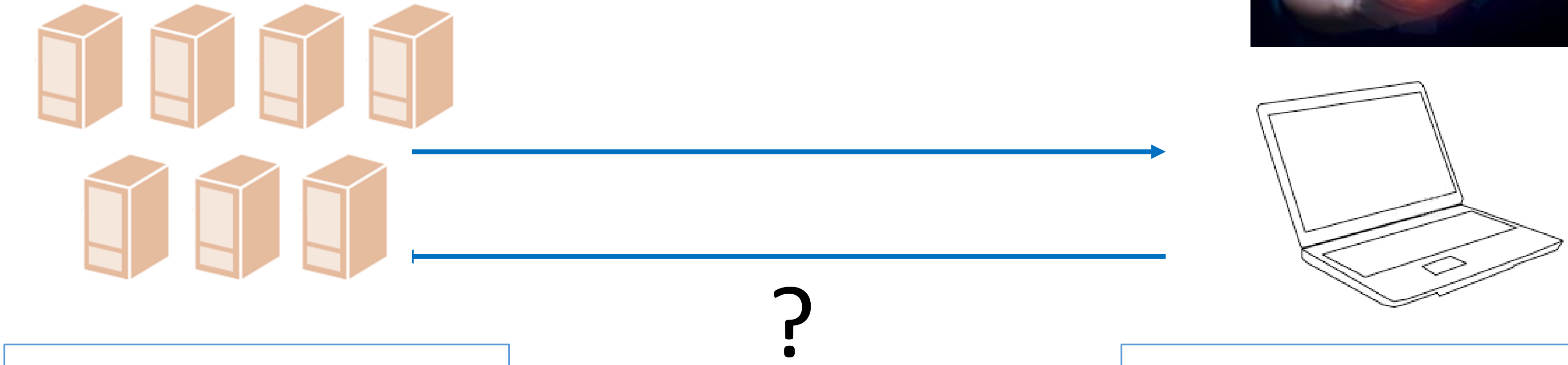
- French Numerical modelling consultancy
- Leader in France of the COMSOL Certified Consultants, key partner worldwide
- 9 members Eng.D. + Ph.D.
- Main partners:
    - big international companies
    - laboratories
- Involved in the Research projects like EU FP (SHARK, SisAl)/ PhD supervision

INNOVATION RADAR
European Commission
SHARK
INDUSTRIALISING LASER FUNCTIONAL TEXTURING
SisAl Pilot

COMSOL
Certified Consultant

markem·imaje
framatome
orano
TDA THALES GROUP
NAVAL GROUP
cea
Continental
MAN
Radiall
GROUPE ADP
ALSTOM
faurecia
AIRBUS
Schlumberger
Nexans
AIR LIQUIDE
SOLVAY asking more from chemistry
ADISSEO A Bluestar Company
fives
L'ORÉAL RECHERCHE
novasep for the life sciences
SORIN GROUP
legrand
Schneider Electric
Parrot

I. Background – Motivations – Objectives



At SIMTEC,

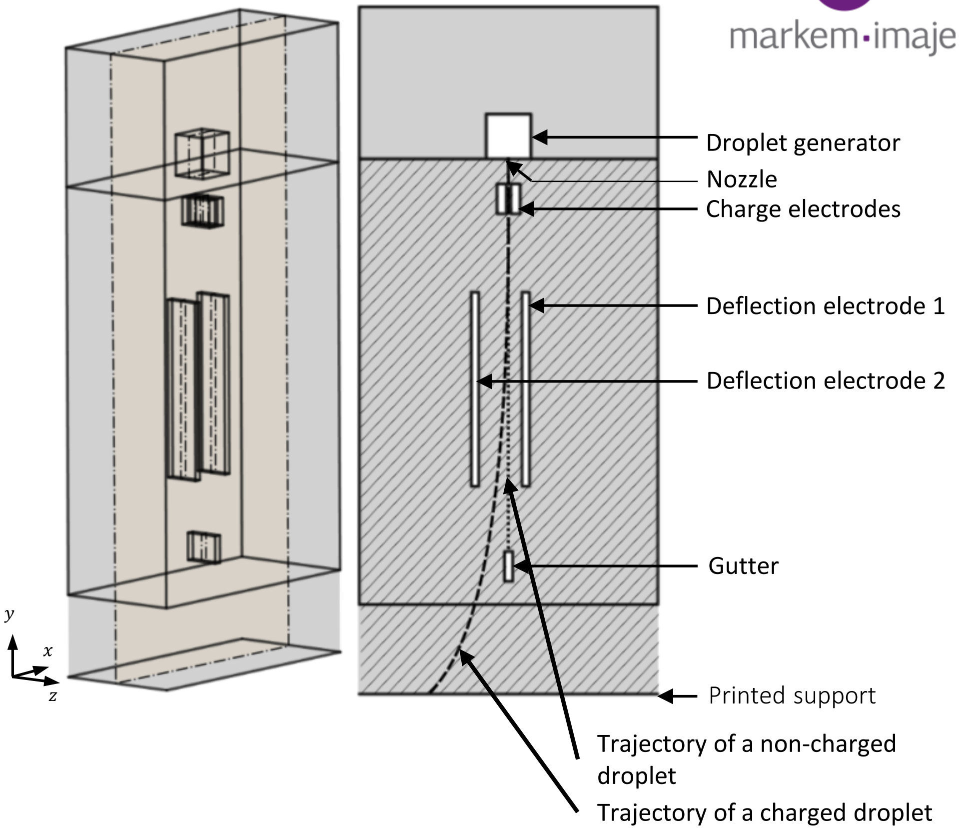
Creation of dozen of COMSOL model every year

Worldwide,

A big boom in AI assisted processes (chatgpt, deepl…)

I. Background – Motivations – Objectives

- Collaboration with MARKEM-IMAJE
- Continuous Inkjet printing (CIJ) : high speed printing for marking and coding
- How does CIJ work?
    - High speed emission of droplets ($\approx 100\ \mathrm{kHz}$ at $\approx 20\ \mathrm{m/s}$)
    - Charge of particular droplets ($\approx 1\ \mathrm{pC}$)
    - Deflection of charged droplets in an electric field ($\approx 1\ \mathrm{kV/mm}$)
    - Impact of charged droplets on the printed support
- Goal: maximizing printing quality
- Printing quality depends on:
    - Breakoff quality at generation
    - Deflection
    - Interactions during flight



Schematic representation of a print head

Tools

→ Data treatments
→ Training models

→ Data generation/collection

Collecting Data

1. Choose a set input values (design of experiment)

→ **Build the "input matrix" in the Python code**

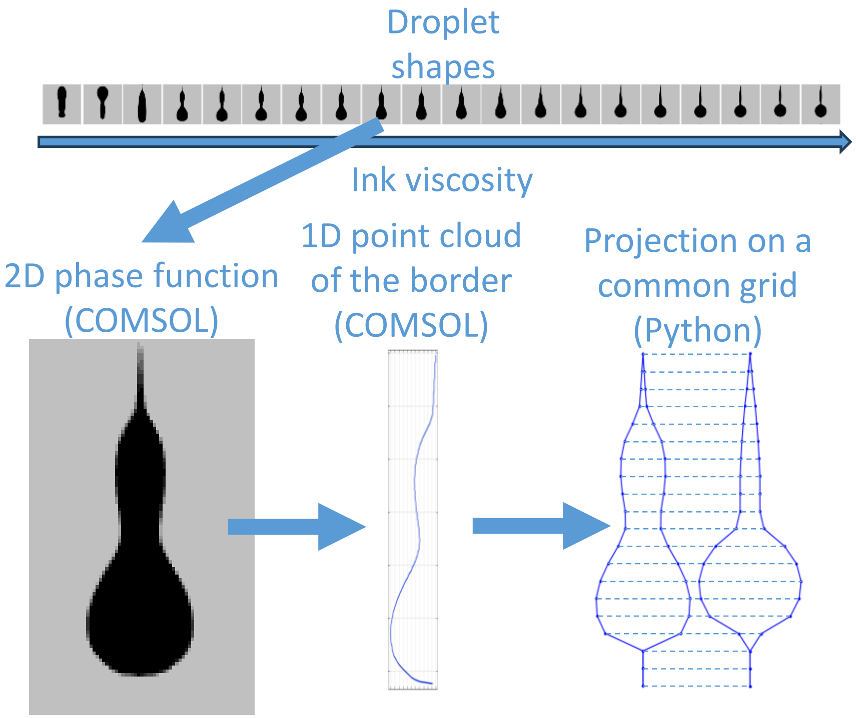
2. Perform one simulation per input value (COMSOL)

3. For each simulation: export the output as a TXT file (COMSOL)

4. Project outputs into a common subspace (COMSOL or Python)

→ **Build the "output matrix" in the Python code**

Use-case



Droplet shapes

Ink viscosity

2D phase function (COMSOL)

1D point cloud of the border (COMSOL)

Projection on a common grid (Python)

Training a Model (Python)

1. Choose a mathematical model to express the viscosity according the radius of the droplet
2. Choose an optimization criterion to train the model
3. Regularization to avoid overfitting

Use-case

Linear model: $\hat{x}_\lambda(y) = \lambda_0 + \sum_i \lambda_i \cdot y_i$

Input prediction

Output

Parameters of the mathematical model to optimize

Optimization criterion: minimization of the MSE

$$J(\lambda) = \sum_j \left[\hat{x}_\lambda(y^j) - x^j\right]^2$$

To minimize

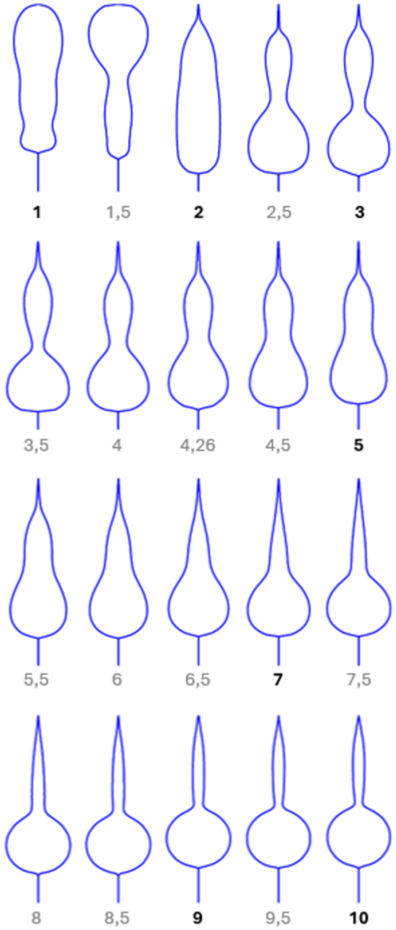
Regularization: LASSO

$$J(\lambda) = \sum_j \left[\hat{x}_\lambda(y^j) - x^j\right]^2 + \alpha \sum_i |\lambda_i|$$

To choose appropriately to prevent overfitting

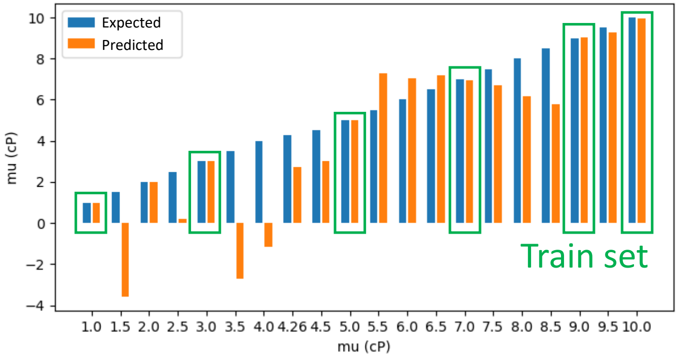
III. Main Results

Dataset: droplets shapes at break simulated for multiple values of viscosities (in cP)



III. Main Results

Figure 2. Performance of the model with a regularization coefficient $\alpha = 10^{-9}$.



- Good fit on *train set*
- Bad predictions on *test set*

→ **Overfitting X**

III. Main Results

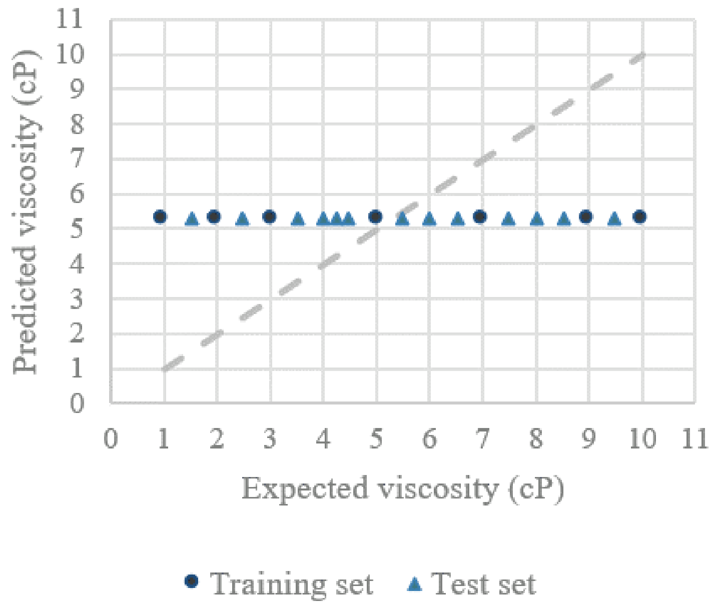
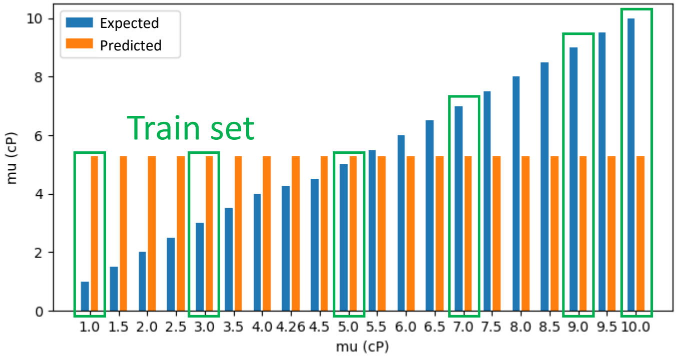


Figure 4. Performance of the model with a regularization coefficient $\alpha = 10^3$.



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→ **Underfitting X**

III. Main Results

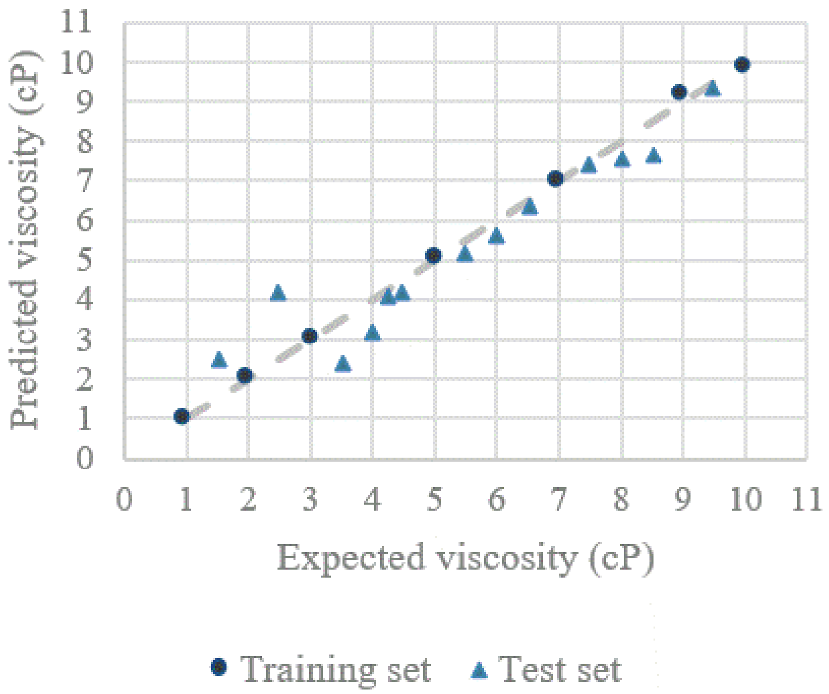
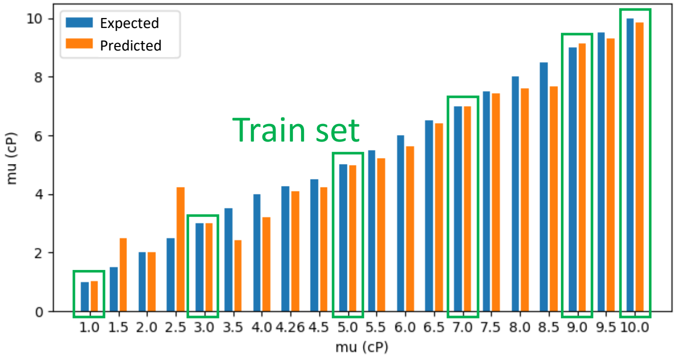


Figure 3. Performance of the model with a regularization coefficient $\alpha = 10^{-1}$.



- Good fit on *train set*
- Good predictions on *test set*

→ **Good model ✓**

IV. Conclusions - Perspectives

- Interest of Machine Learning methods:
    - Minimize the simulation computational cost → Building **Surrogate Models**
    - Retrieve simulation inputs providing a given output → Solving **Inverse Problems**

- What we have done:
    1. Extract inputs/outputs data from COMSOL
    2. Solve an inverse problem using Supervised Machine Learning tools in Python

- Flexibility of COMSOL is of great help to do so ☺

→ **Coupling COMSOL with Machine Learning tools is feasible!**

To finish…

Thank you!

Q&A?

Our question: Who would like to try on your models? ☺

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