Informed and augmented learning for the efficient simulation of complex systems

Francisco (Paco) CHINESTA

Agenda

1. Contexte
2. Méthodes
3. Applications

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1. Contexte
2. Méthodes
3. Applications

21st century engineering:

- From design to operation

- From component to system of systems

The Twin Continuum

VIRTUAL

- 100% Physics
- U=U(F)
- Software

- Processing time
- Resources
- Complex systems
- Variability
- Uncertainty

INFORMED

u(x) AI-based such that L(u)=G

AUGMENTED - HYBRID

$u(x)=u^P(x)+u^D(x)$

- Less data
- Faster
- Explainable

DIGITAL

- Unknown or poor model
- Ui,Fi, i=1,2, …
- Machine learning: U(F)

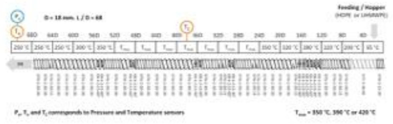
- Data cost
- Which data, where & when?
- Extrapolation
- Explanation

Agenda

1. Contexte
2. Méthodes
3. Applications

I – Data Typology

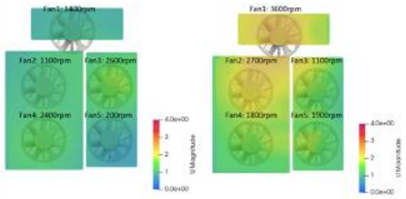
Lists



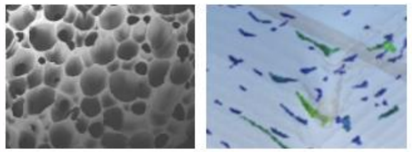
Process Inputs				Extrusion in-Line Measurements				
PE Type	Q (kg/h)	N (rpm)	T_{max} (°C)	Torque (N.m)	Pe (Bar)	Tc (°C)	Engine Power (kW)	Te (°C)
HDPE	3	300	350	21.3	28	355	1.04	248
HDPE	3	600	350	17.7	22	357	1.68	273
HDPE	6	300	350	13.8	12	353	3.97	236
HDPE	6	600	350	12.4	12	355	6.89	258
HDPE	1	300	390	10.3	7	395	0.46	226
HDPE	3	300	390	16.7	13	395	0.81	242
HDPE	3	300	390	17.4	17	393	0.81	247
HDPE	3	500	390	16.0	15	394	1.23	260
HDPE	3	500	390	16.0	15	394	1.20	261
HDPE	3	600	390	13.8	12	395	1.31	263
HDPE	3	700	390	14.2	14	396	1.59	268
HDPE	3	1000	390	12.4	8	397	2.01	274
HDPE	5	600	390	20.6	18	396	2.01	276
HDPE	6	300	390	28.7	25	391	0.69	273
HDPE	6	600	390	21.3	19	393	1.02	286
HDPE	6	1000	390	17.0	20	396	0.38	307
HDPE	3	300	420	12.4	4	423	0.60	226
HDPE	3	600	420	10.3	3	424	1.00	230
HDPE	6	300	420	24.8	10	421	0.59	257
HDPE	6	600	420	19.2	8	422	1.81	258
UHMWPE	1	300	390	13.1	25	397	0.64	260
UHMWPE	1	600	390	11.4	13	398	1.09	276
UHMWPE	1	1000	390	9.6	9	399	1.38	286
UHMWPE	3	400	390	22.0	35	398	1.41	280
UHMWPE	3	600	390	16.3	30	397	1.74	307
UHMWPE	3	1000	390	14.2	34	397	1.74	307
UHMWPE	3	300	420	21.3	10	424	1.00	234
UHMWPE	3	600	420	11.0	9	430	1.06	256
UHMWPE	3	1000	420	10.3	7	430	1.61	268

Images

FEM

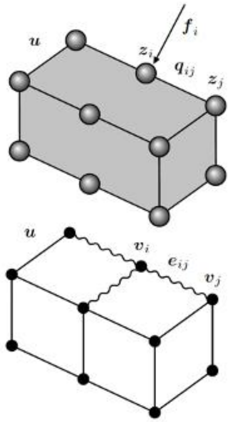


EXP



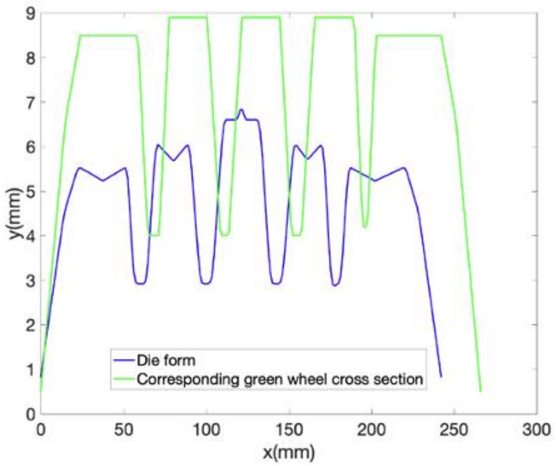
Descriptors, metrics & data transformation

Graphe

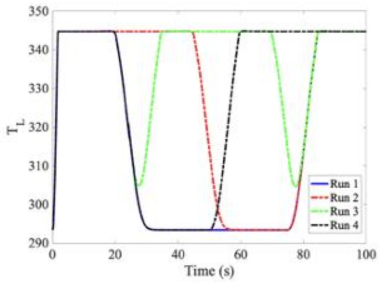


Connectivity, balance & behavior

Curves



Time series

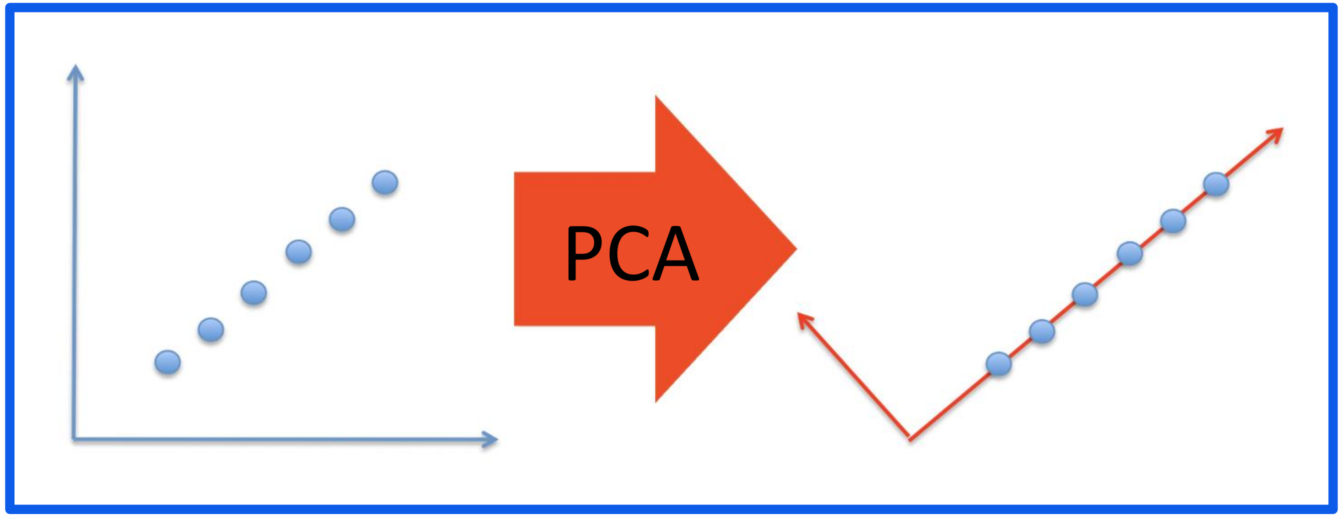


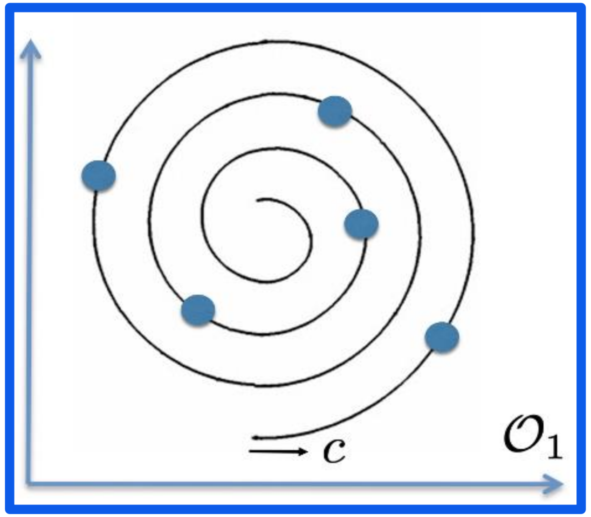
Causality, stability description and metrics

- ❑ Volume
- ❑ Useful versus useless
- ❑ Completeness

I – Data Reduction

LINEAR

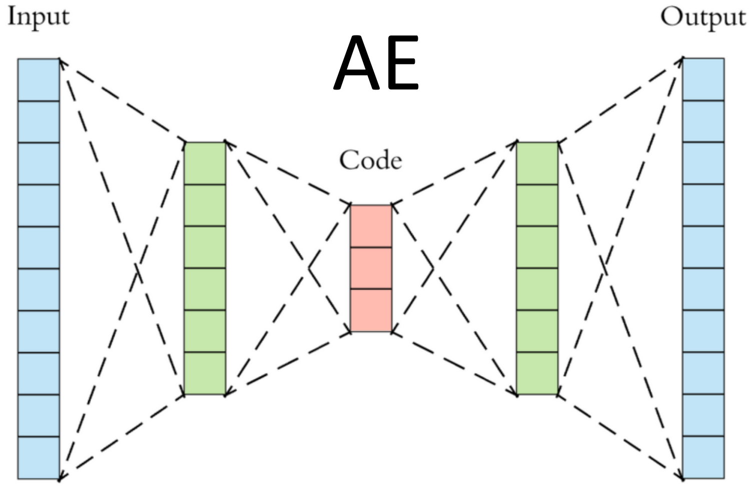




Manifold Learning

NONLINEAR

AE



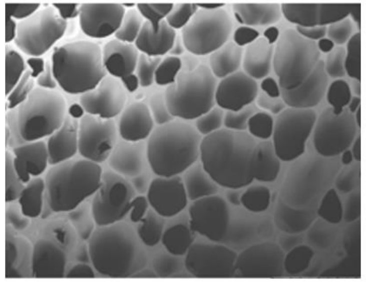
$$\mathcal{L}(\mathbf{y},\mathbf{y}') = \|\mathbf{y}-\mathbf{y}'\|^2 = \|\mathbf{y}-\sigma'(\mathbf{W}'(\sigma(\mathbf{W}\mathbf{y}+\mathbf{b}))+\mathbf{b}')\|^2$$

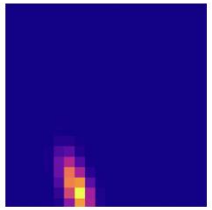
I – Data: Metrics

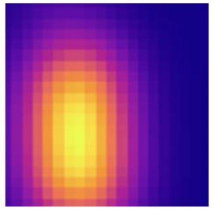
Topological Data Analysis - TDA

Time series

Complex images



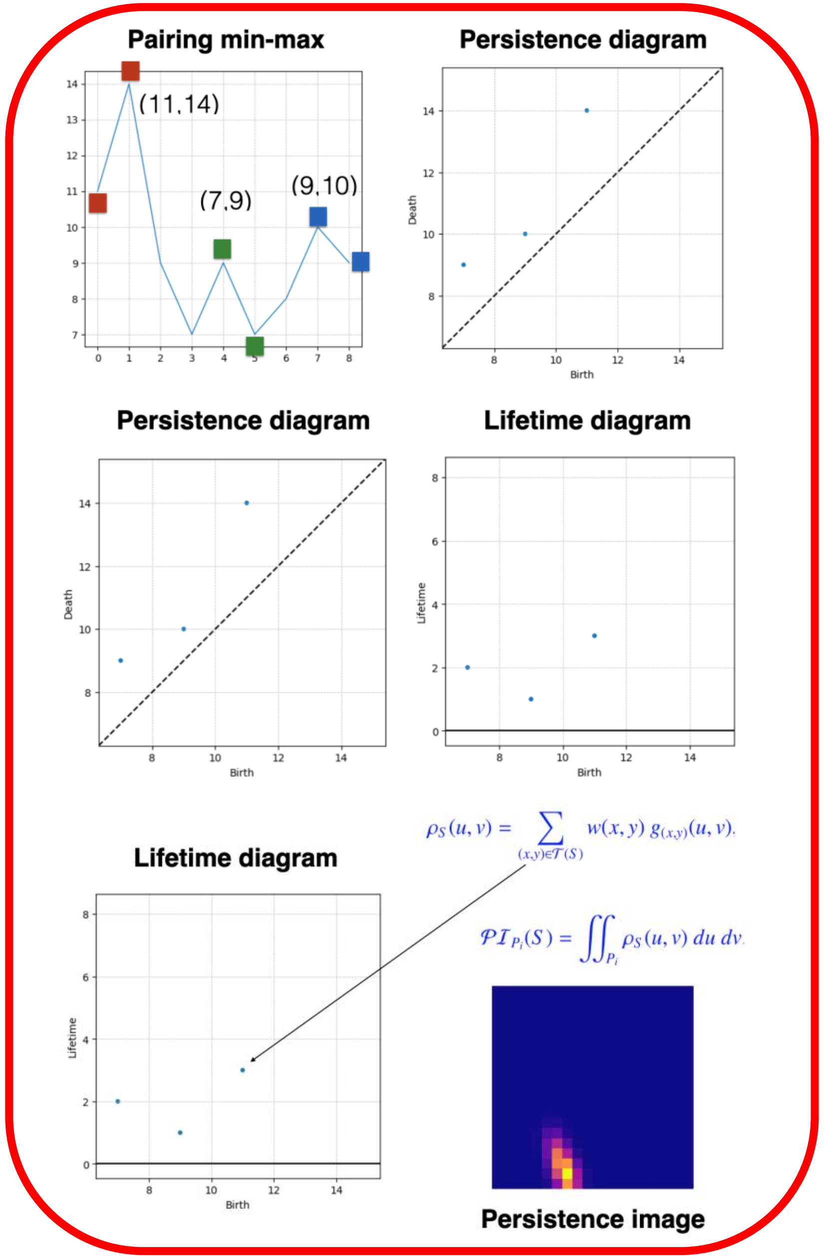


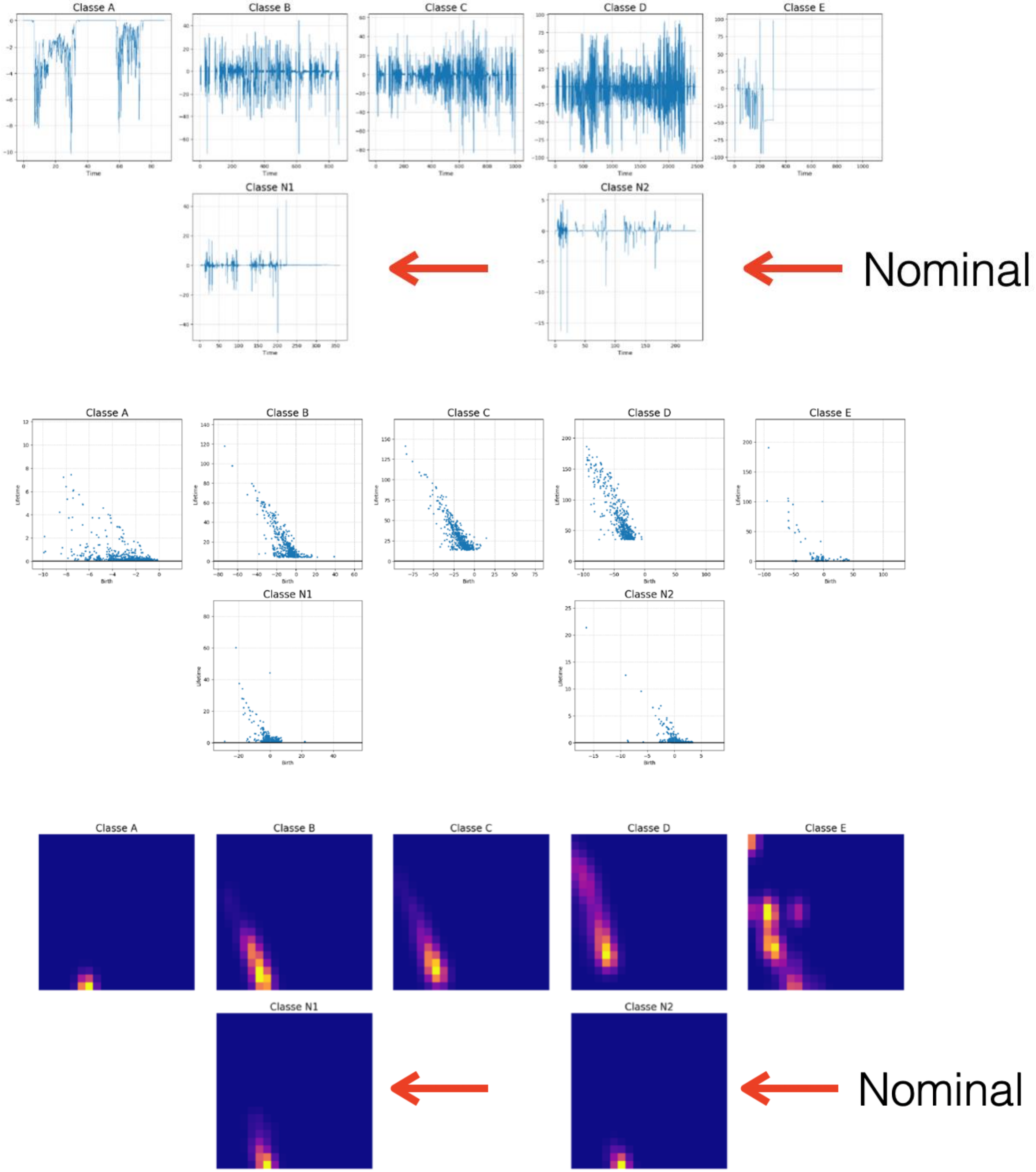


A sort of goal oriented

QR code / Passport

BUT in a vector space


Pairing min-max
(11,14)
(7,9)
(9,10)
Persistence diagram
Death
Birth
Persistence diagram
Lifetime diagram
Lifetime
$\rho_S(u,v) = \sum_{(x,y)\in \mathcal{T}(S)} w(x,y)\, g_{(x,y)}(u,v).$
Lifetime diagram
$\mathcal{PI}_{P_i}(S) = \iint_{P_i} \rho_S(u,v)\, du\, dv.$
Persistence image

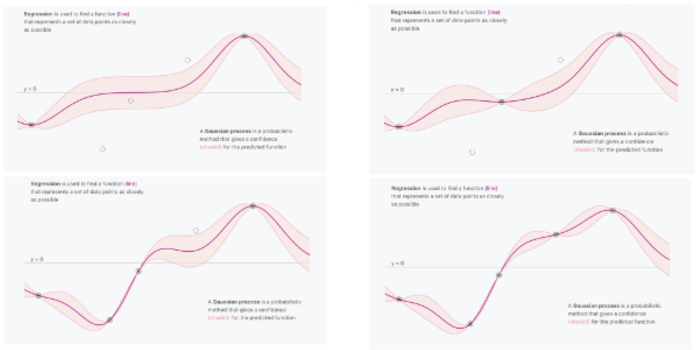

Classe A
Classe B
Classe C
Classe D
Classe E
Classe N1
Classe N2
Nominal
Time
Birth
Lifetime
Classe A
Classe B
Classe C
Classe D
Classe E
Classe N1
Classe N2
Classe A
Classe B
Classe C
Classe D
Classe E
Classe N1
Classe N2
Nominal

I – Data: Active learning

Gaussian processes

$$y_A | y_B = y_B \sim \mathcal{N}(\mu_A + \Sigma_{AB}\Sigma_{BB}^{-1}(y_B - \mu_B), \Sigma_{AA} - \Sigma_{AB}\Sigma_{BB}^{-1}\Sigma_{BA})$$

$$f_* | (Y_1 = y_1, \dots, Y_n = y_n, \mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}_t) \sim \mathcal{N}(K_*^\top K^{-1} y, K_{**} - K_*^\top K^{-1} K_*)$$

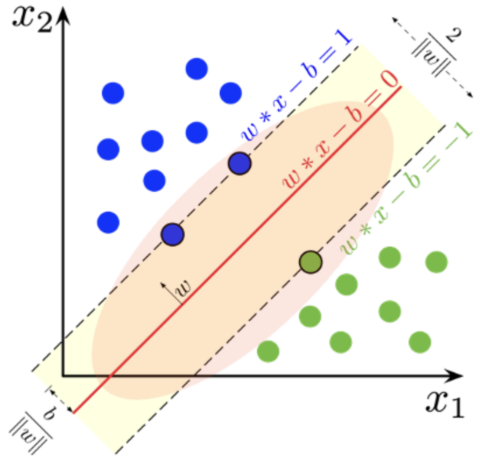


MD
&
QoI

Classification

Entropy-based
sampling

SVM



Physics informed

$$u(x, \mu_1, \dots, \mu_P) \approx \sum_{i=1}^{N} X_i(x) M_i^1(\mu_1) \cdots M_i^P(\mu_P)$$

$$X_i(x), i = 1, \dots, N$$

DEIM

Physics augmented

$$(\mathbf{K} + \Delta\mathbf{K})(\mathbf{U} + \Delta\mathbf{U}) = \mathbf{F}$$

$$\Delta\mathbf{U} = (\mathbf{K} + \Delta\mathbf{K})^{-1}\mathbf{F} - \mathbf{U}$$

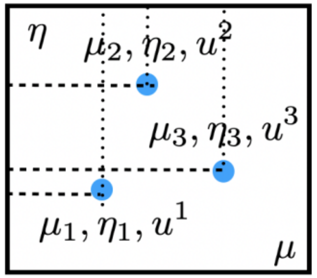
$$\hat{x}_{\Delta\mathbf{K}} = \mathbf{X}_j \rightarrow \mathtt{max}_j |\Delta U_j|$$

II – Modelling from data

- Fundamental laws:
  - Mass, Momentum, Energy, … conservation
  - Entropy production
  - Objectivity
- Conservation vs symmetries:
  - Noether theorem
- Other properties:
  - Stability, Convexity, …
- Phenomenological constitutive equations

II – Modelling from data

LINEAR



Linear approximation

$$u(\mu, \eta) = a + b\mu + c\eta$$

Beyond linear approximations

$$[1, \mu, \eta, \mu^2, \mu\eta, \eta^2, \mu^2\eta, \mu^2\eta^2, \mu\eta^2]$$

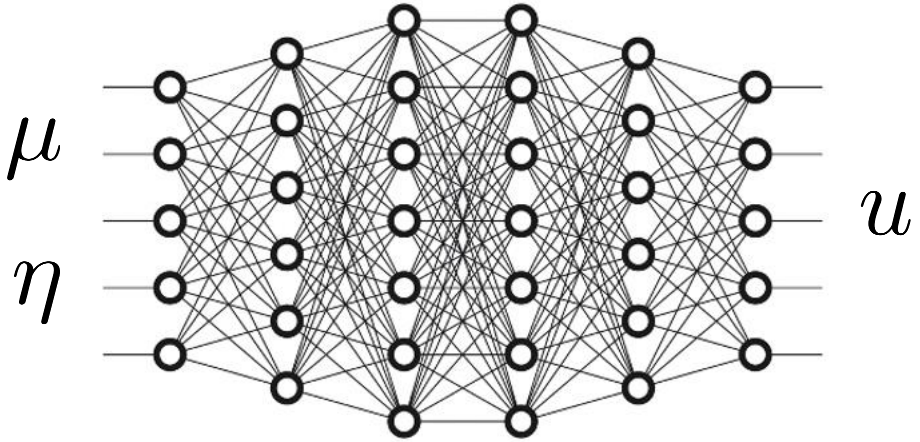
$$u(\mu, \eta) = \sum_{i=1}^{N} c_i \mathcal{F}_i(\mu, \eta)$$

Regularization by sparsity

$$\sum_{j=1}^{3} \|u(\mu_j, \eta_j) - u^j\|_2^2 + \lambda \sum_{i=1}^{N} |c_i|$$

Regularized Polynomial Regression -**RPR**-

NONLINEAR



Nonlinear Regression -**NLR**-

II – Remark: Regression/Approximation

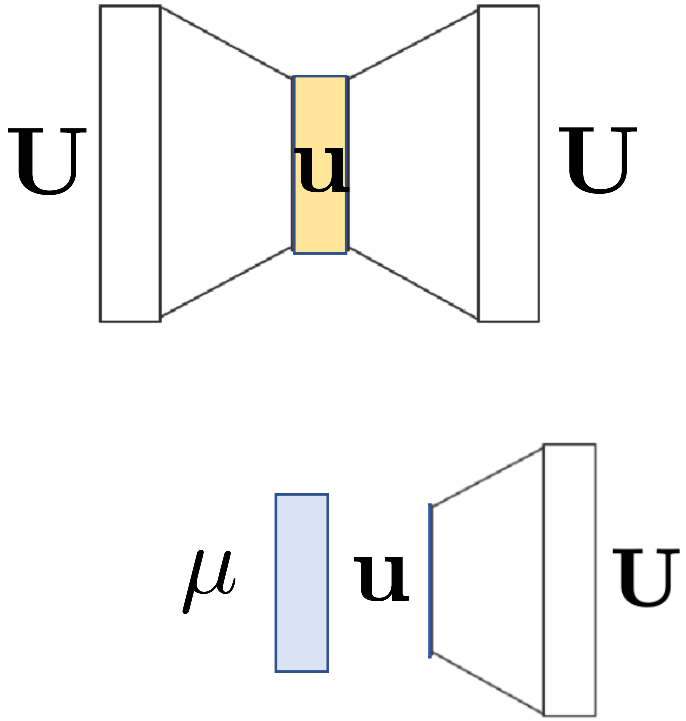
Linear regression-based linear approximation:

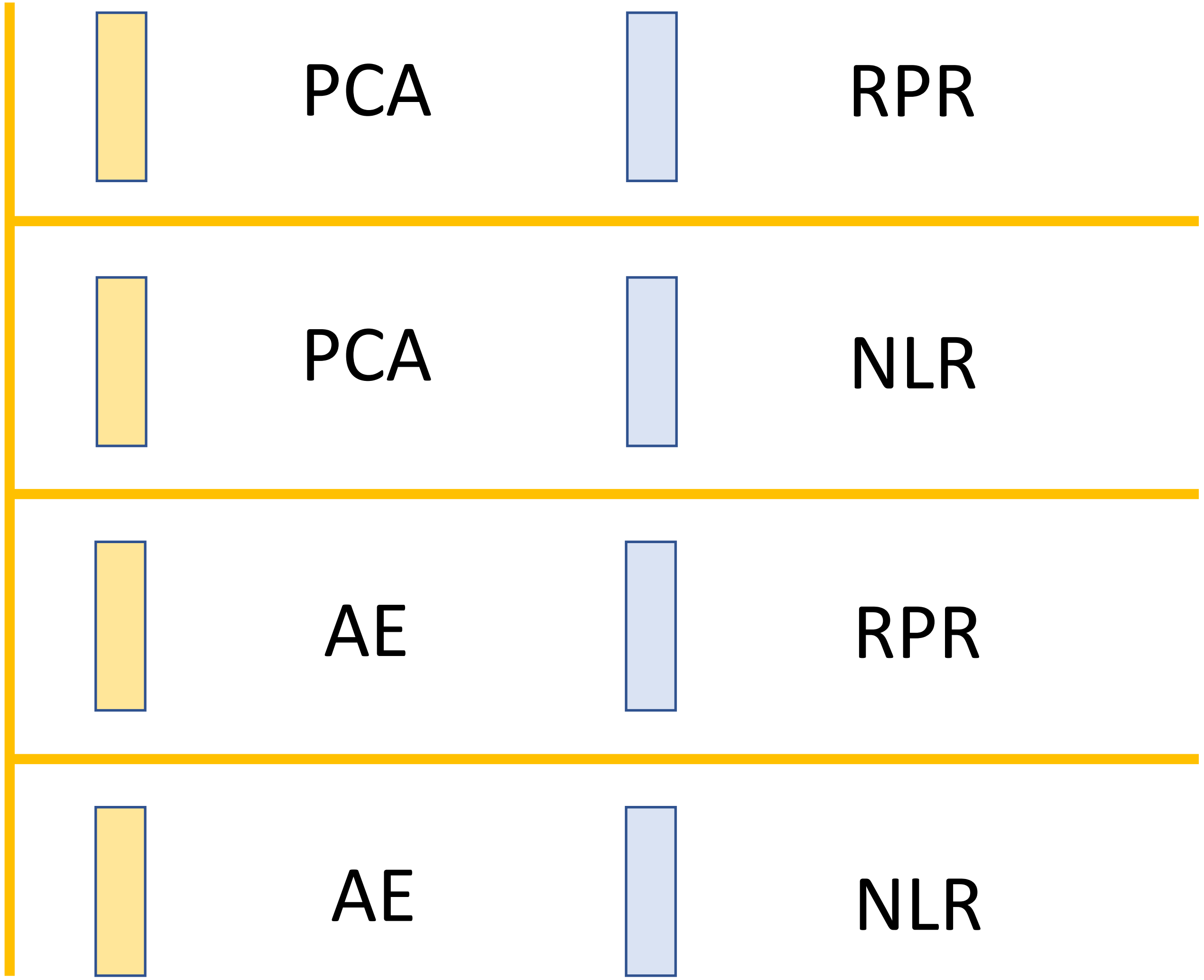
$$u = a + b\mu + c\eta$$

Linear regression-based nonlinear approximation:

$$u = a + b\mu + c\eta + d\mu\eta + e\mu^2 + \ldots$$

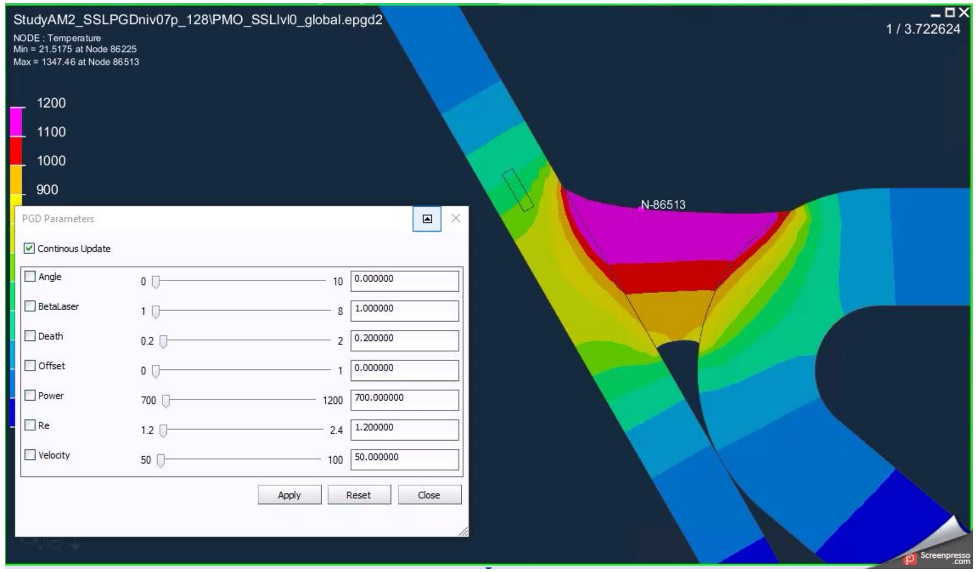
II – Modelling at the latent space

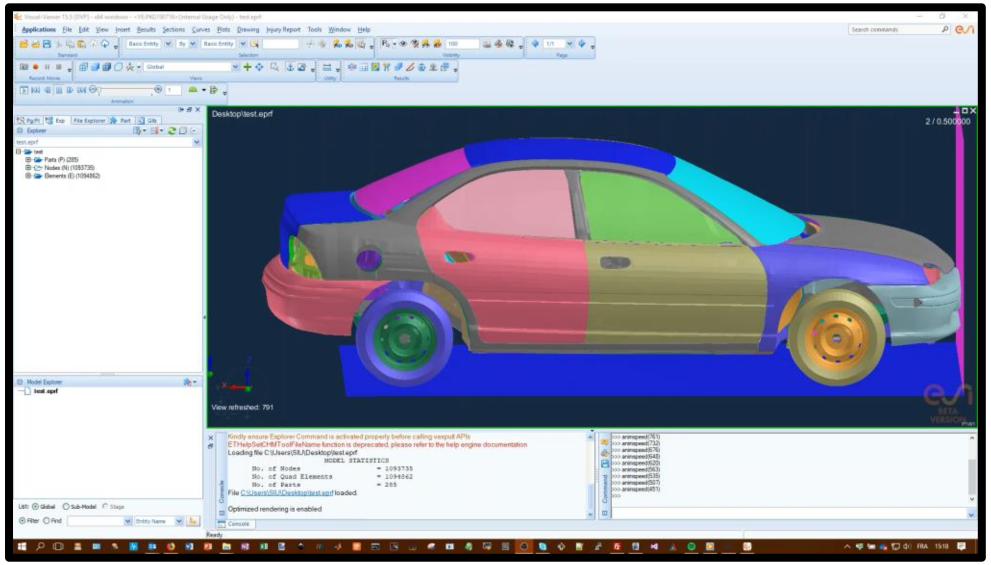


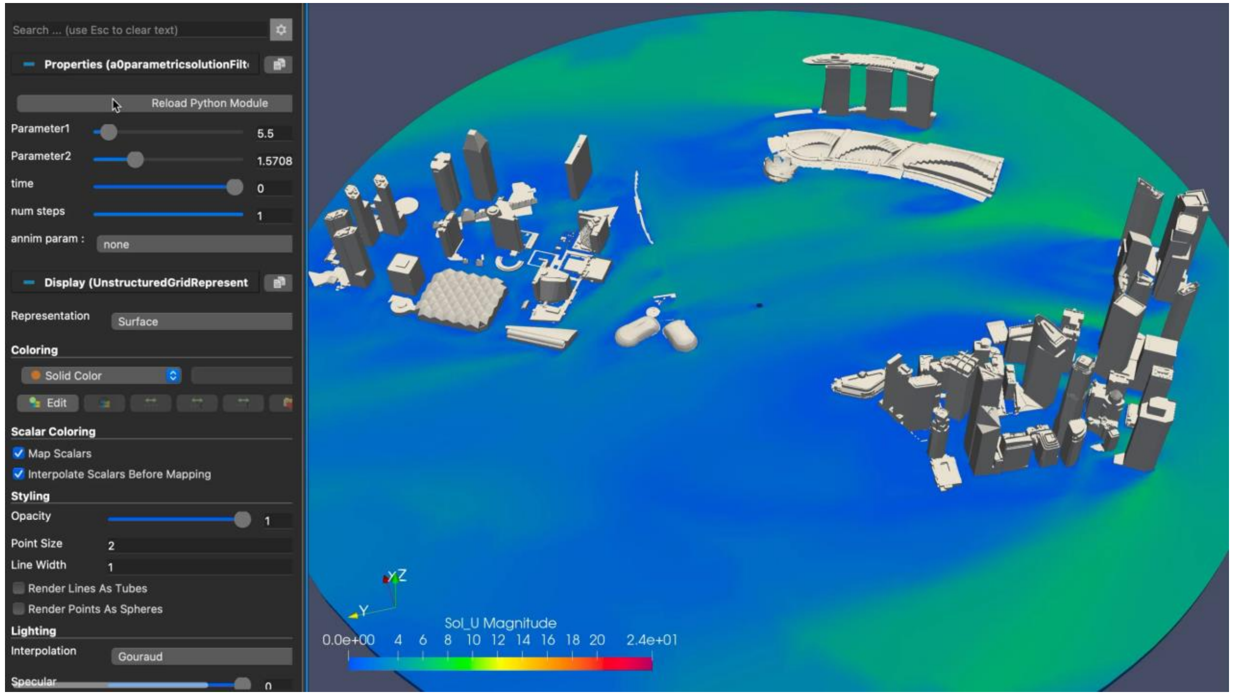


II – Linear-Linear

PCA RPR



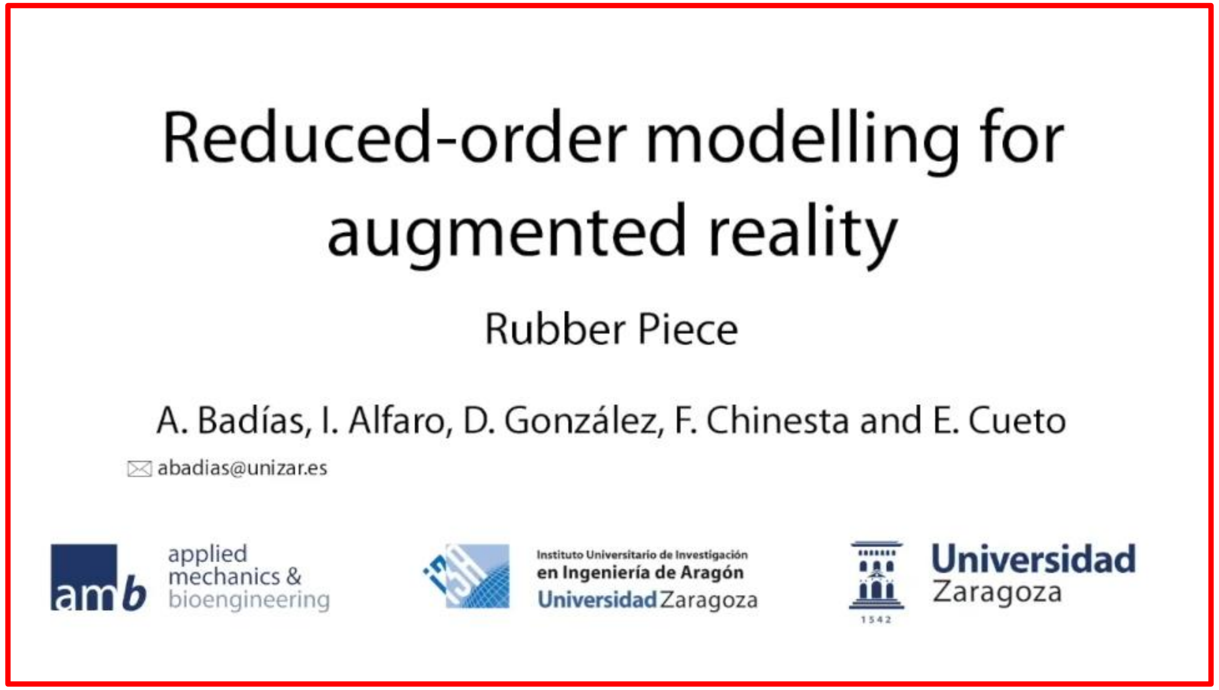




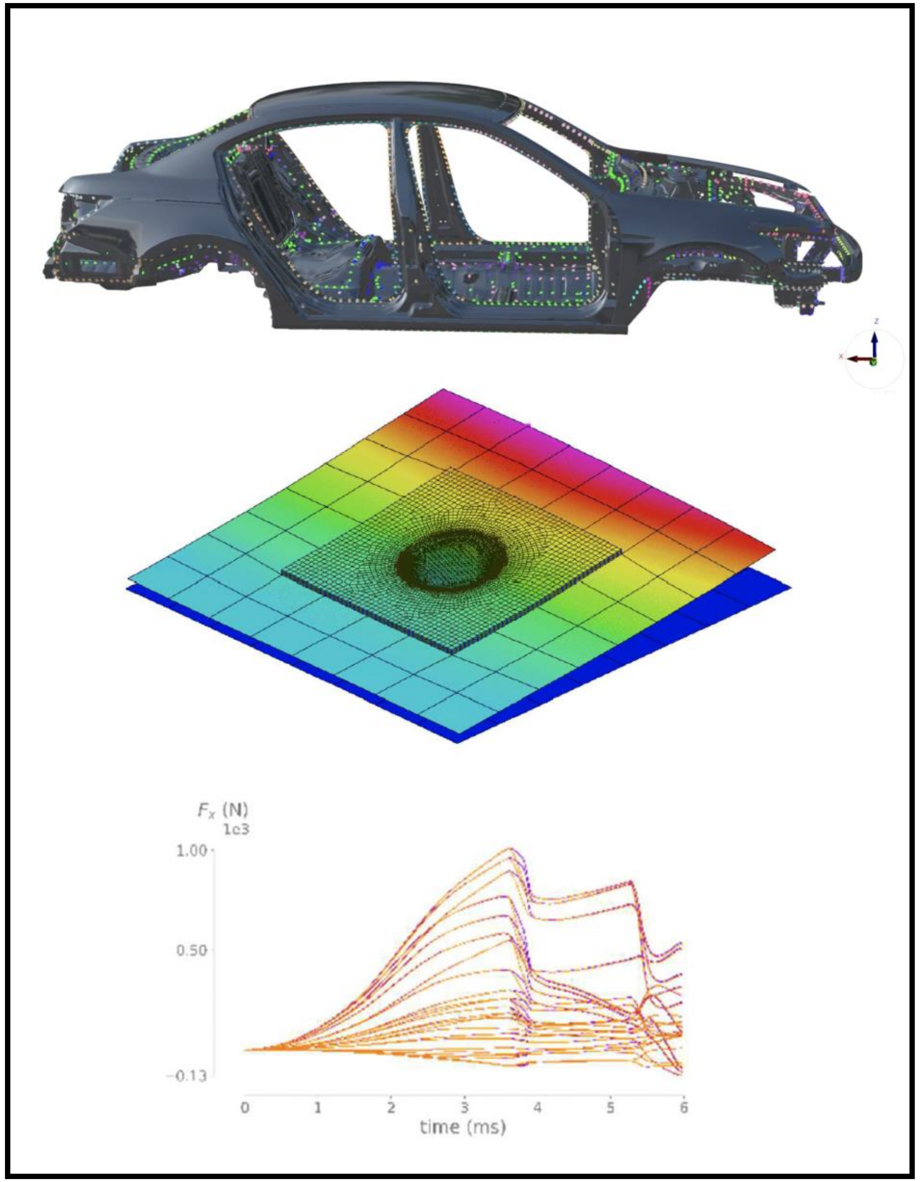
DesCartes

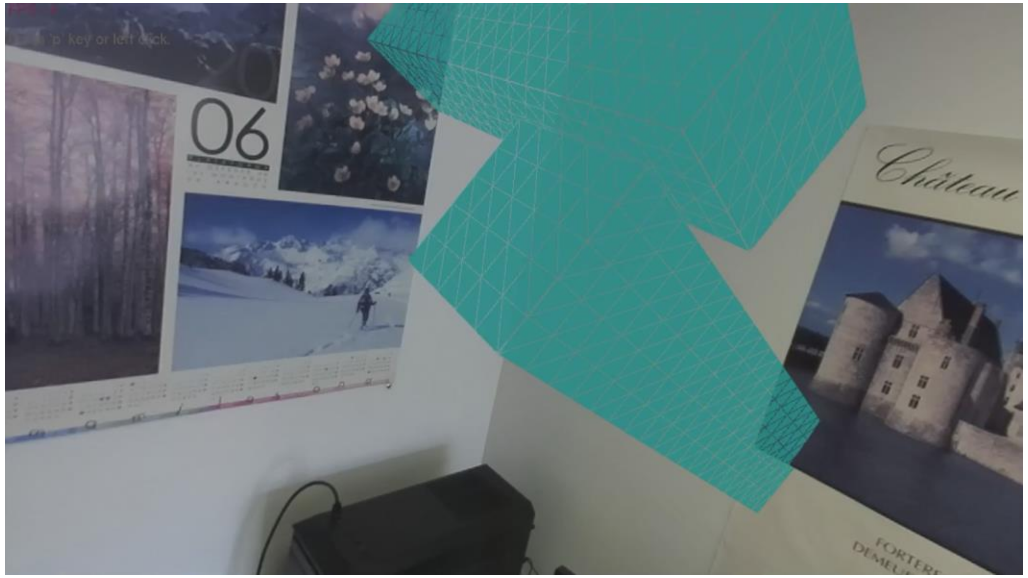
II – Linear-Linear

PCA RPR



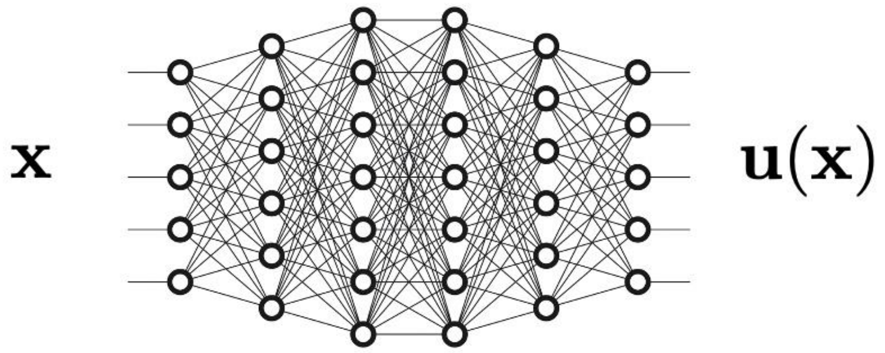
II – Nonlinear-Nonlinear





III – Hybridation

Physics-informed



$$\text{Loss} = \|\mathcal{L}(\mathbf{u}) - \mathcal{F}(\mathbf{x})\| + \text{BC}$$

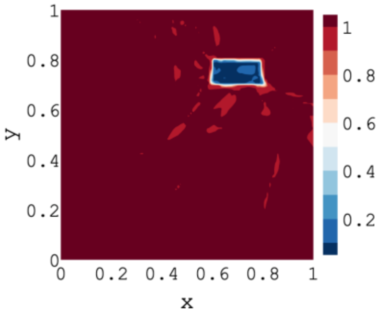
+ DATA

Physics-Augmented: Physics-based + Data-driven

IV - Numerical technologies

- Regularized polynomial regressions, GP, DT, RF, SVR, …
- CNN
- GNN
- rNN, LSTM, ResNET, NeuralODE, DeepONet, Reservoir computing, …
- GAN
- Transformers
- Autoencoders
- PINN, SPNN, PANN, …

PINN



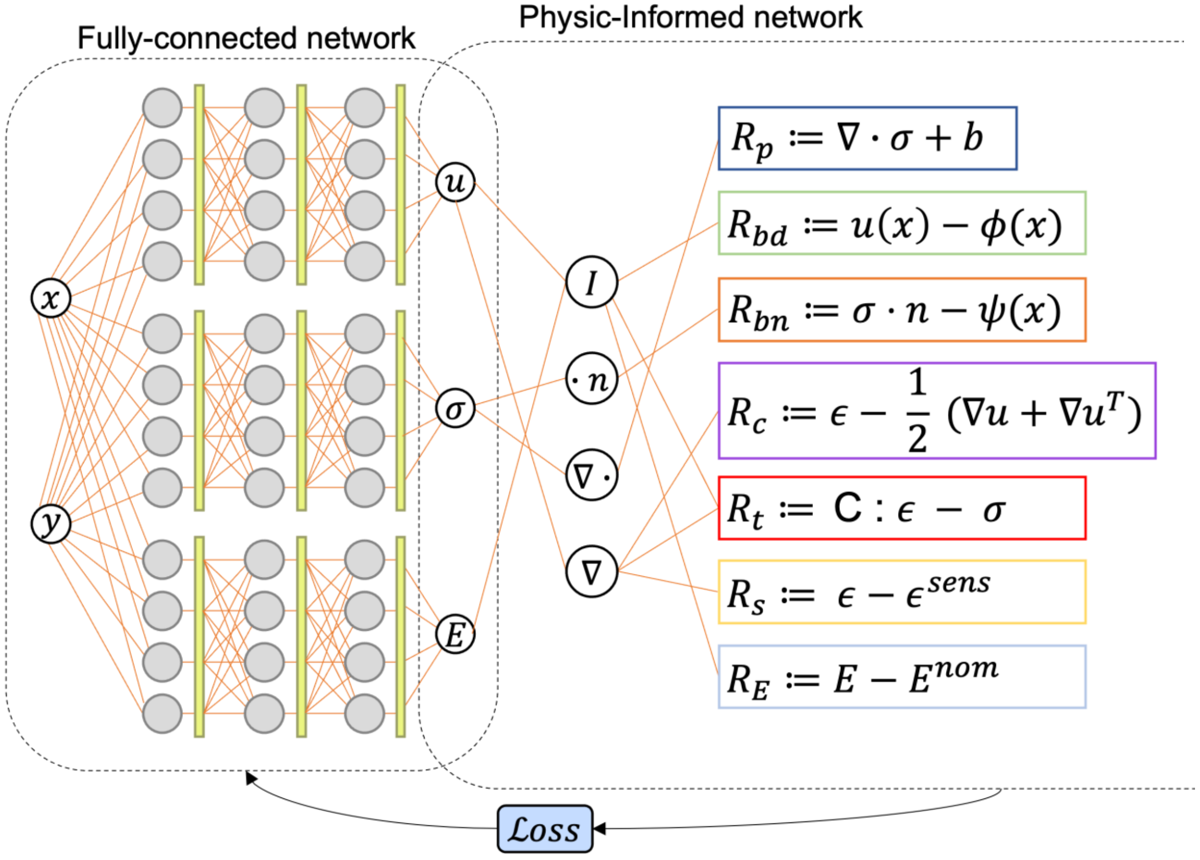
$$\mathcal{L}_d = \frac{1}{N_d}\sum_{i}^{N_d}\left|\boldsymbol{\nabla}\cdot\hat{\sigma}(\mathbf{x}^i) - \mathbf{b}(\mathbf{x}^i)\right|^2$$

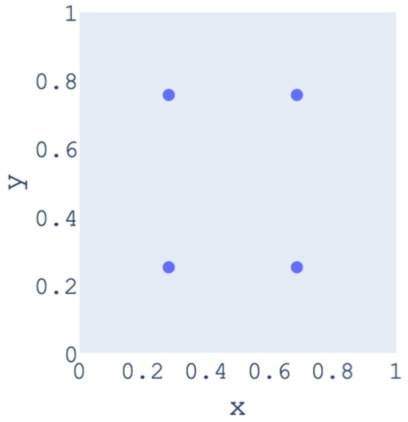
$$\mathcal{L}_b = \frac{1}{N_{dc}}\sum_{j}^{N_{dc}}\left|\hat{u}(\mathbf{x}^j) - \phi(\mathbf{x}^j)\right|^2 + \frac{1}{N_{nn}}\sum_{l}^{N_{nn}}\left|\hat{\sigma}(\mathbf{x}^l)\cdot\mathbf{n} - \psi(\mathbf{x}^l)\right|^2$$

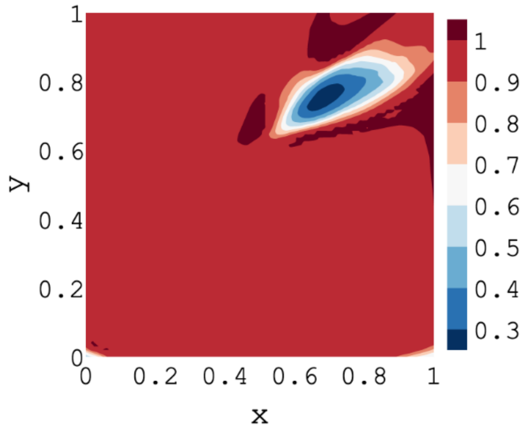
$$\mathcal{L}_f = \frac{1}{N_d}\sum_{i}^{N_d}\left|\hat{\sigma}(\mathbf{x}^i) - C:\epsilon(\mathbf{x}^i)\right|$$

$$\mathcal{L}_{dat} = \frac{1}{N_{sens}}\sum_{j}^{N_{sens}}\left|\epsilon(\mathbf{x}^j) - \epsilon^{sens}(\mathbf{x}^j)\right|^2$$

$$\mathcal{L}_c = \frac{1}{N_d}\sum_{i}^{N_d}\left|\hat{E}(\mathbf{x}^i) - E^{nom}(\mathbf{x}^i)\right|$$







TINN

$$\dot{\boldsymbol{z}}_t = \boldsymbol{L}(\boldsymbol{z}_t)\nabla E(\boldsymbol{z}_t) + \boldsymbol{M}\nabla S(\boldsymbol{z}_t), \quad \boldsymbol{z}(0) = \boldsymbol{z}_0$$

Poisson matrix: reversibility

Friction matrix: irreversibility

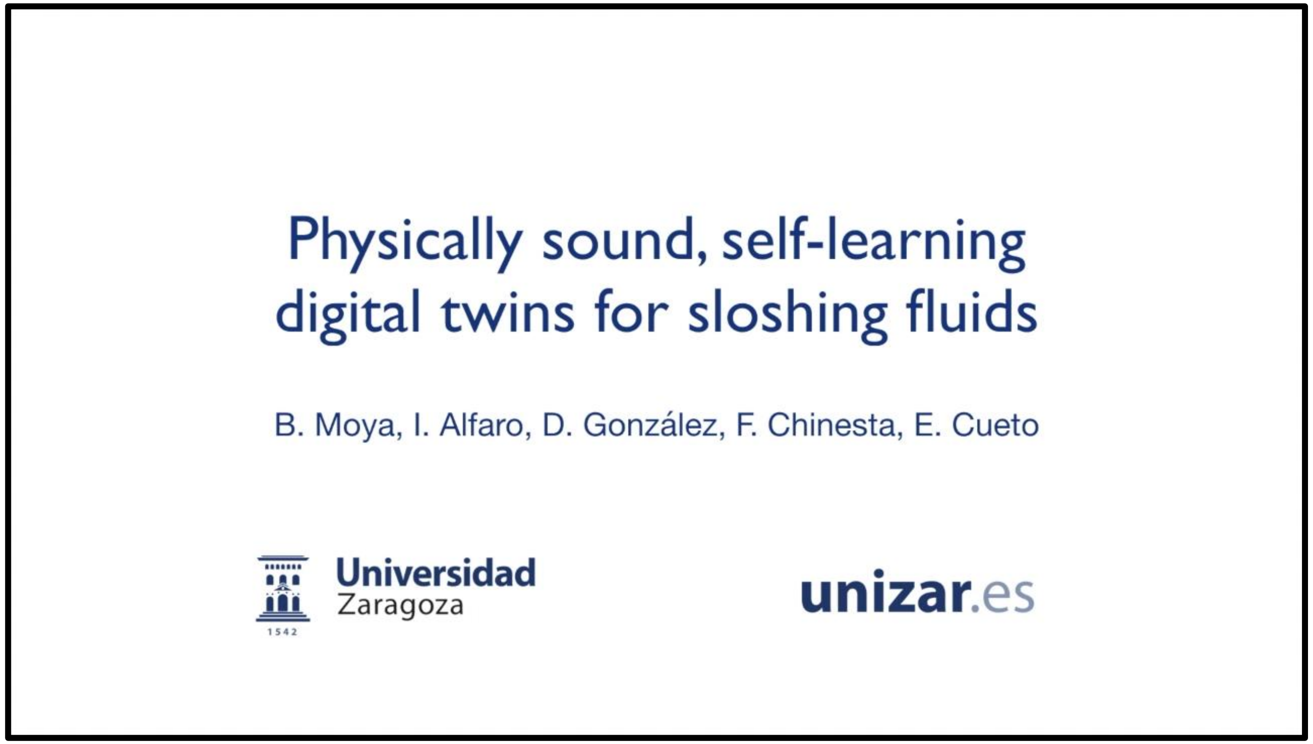
with

$$\boldsymbol{L}(\boldsymbol{z}) \cdot \nabla S(\boldsymbol{z}) = \boldsymbol{0},$$
$$\boldsymbol{M}(\boldsymbol{z}) \cdot \nabla E(\boldsymbol{z}) = \boldsymbol{0}.$$

$$\frac{\boldsymbol{z}_{n+1} - \boldsymbol{z}_n}{\Delta t} = \mathsf{L}(\boldsymbol{z}_{n+1}, \boldsymbol{z}_n)\mathsf{DE}(\boldsymbol{z}_{n+1}, \boldsymbol{z}_n) + \mathsf{M}(\boldsymbol{z}_{n+1}, \boldsymbol{z}_n)\mathsf{DS}(\boldsymbol{z}_{n+1}, \boldsymbol{z}_n)$$

$$\boldsymbol{\mu} = \{\mathsf{L}, \mathsf{M}, \mathsf{DE}, \mathsf{DS}\} = \underset{\boldsymbol{\mu}*}{\arg\min} ||\boldsymbol{z}(\boldsymbol{\mu}) - \boldsymbol{z}^{\mathtt{meas}}||$$

with
$$\mathsf{DE} = \boldsymbol{A}\boldsymbol{z}$$
$$\mathsf{DS} = \boldsymbol{B}\boldsymbol{z}$$



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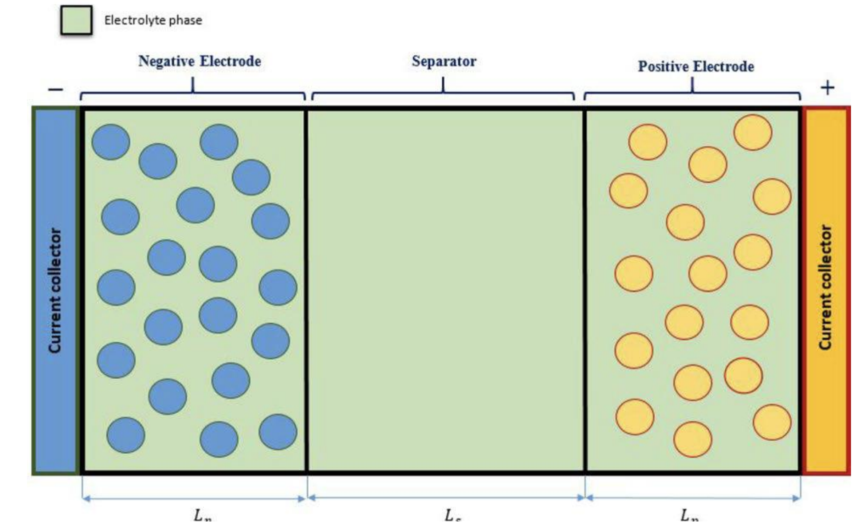
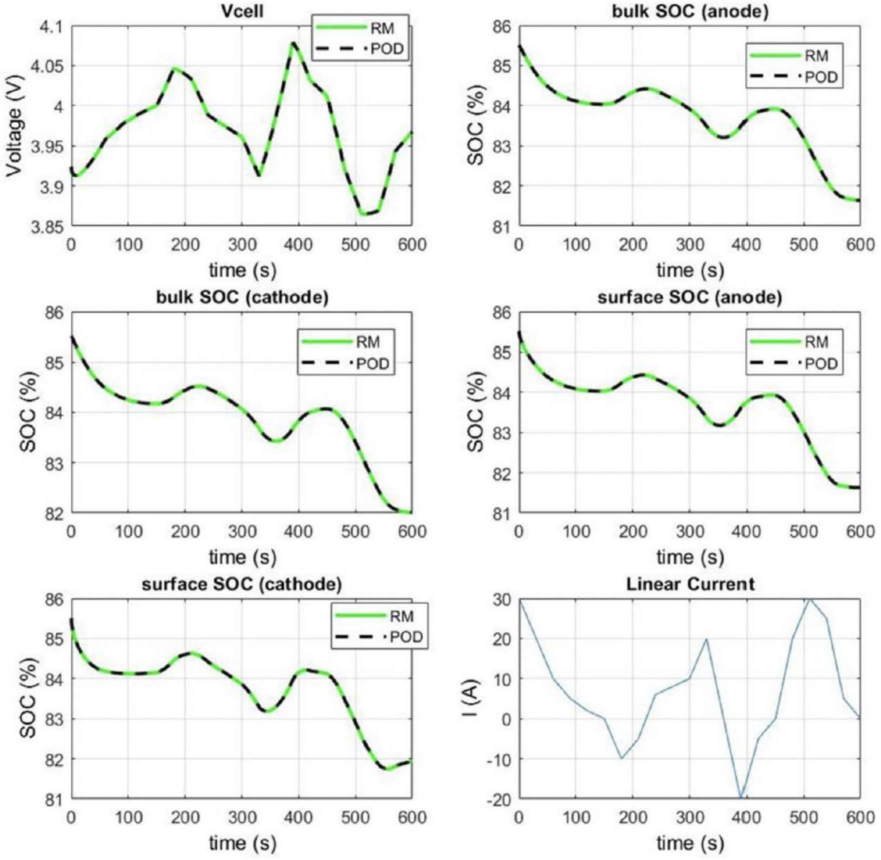
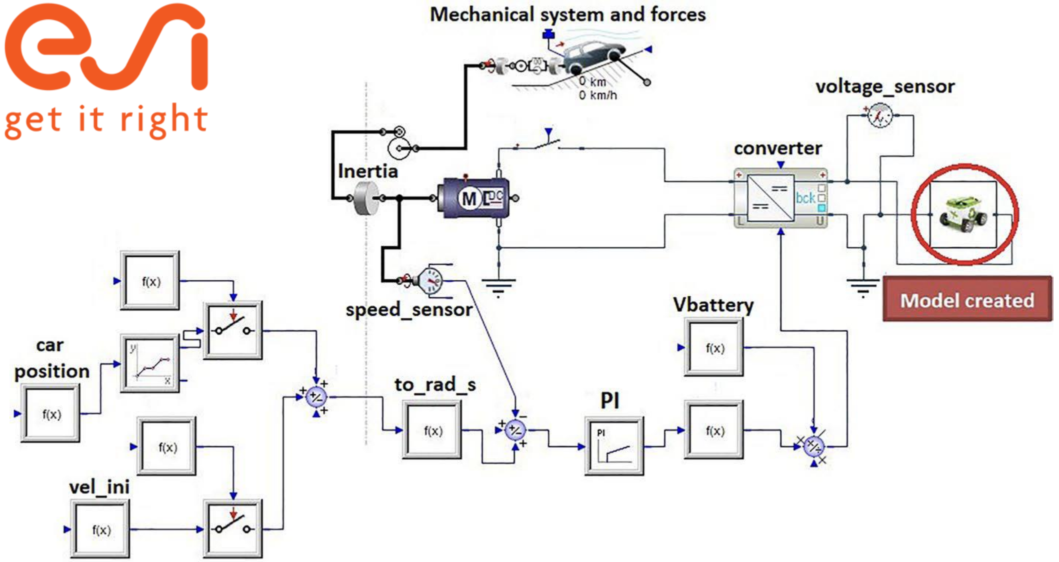
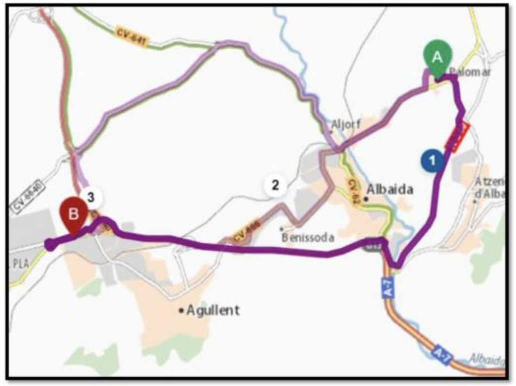
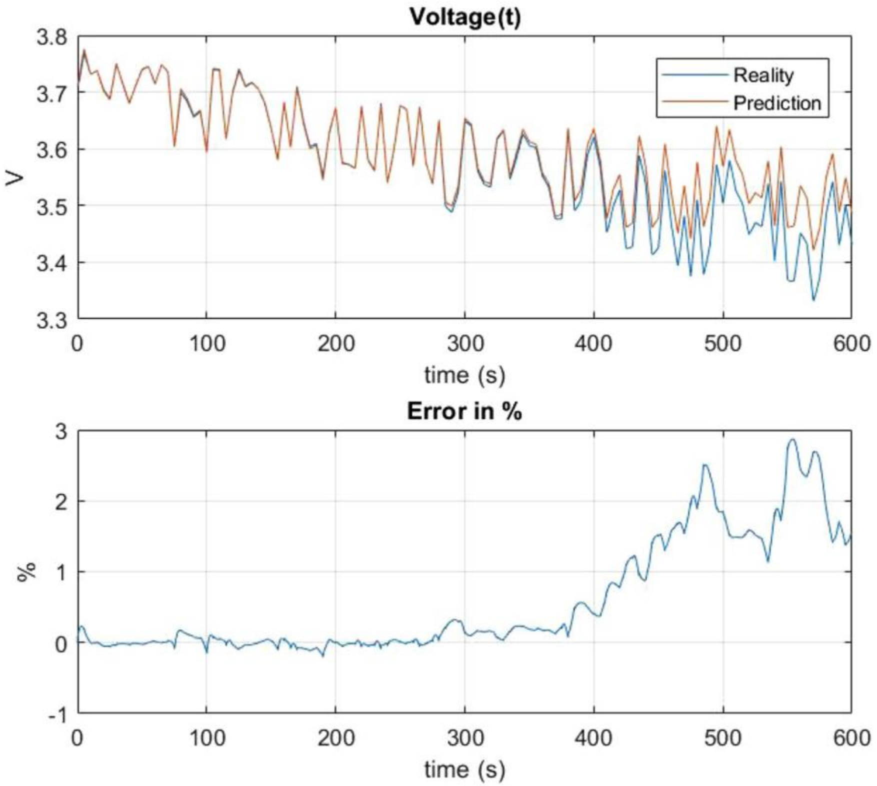




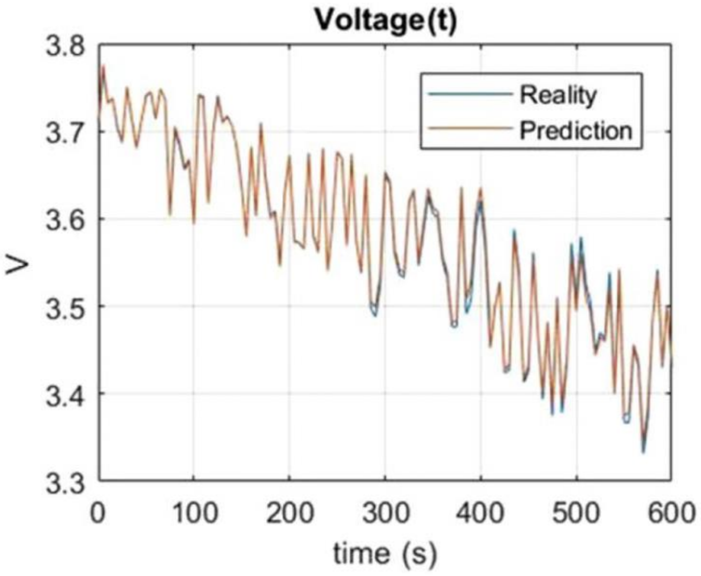
get it right



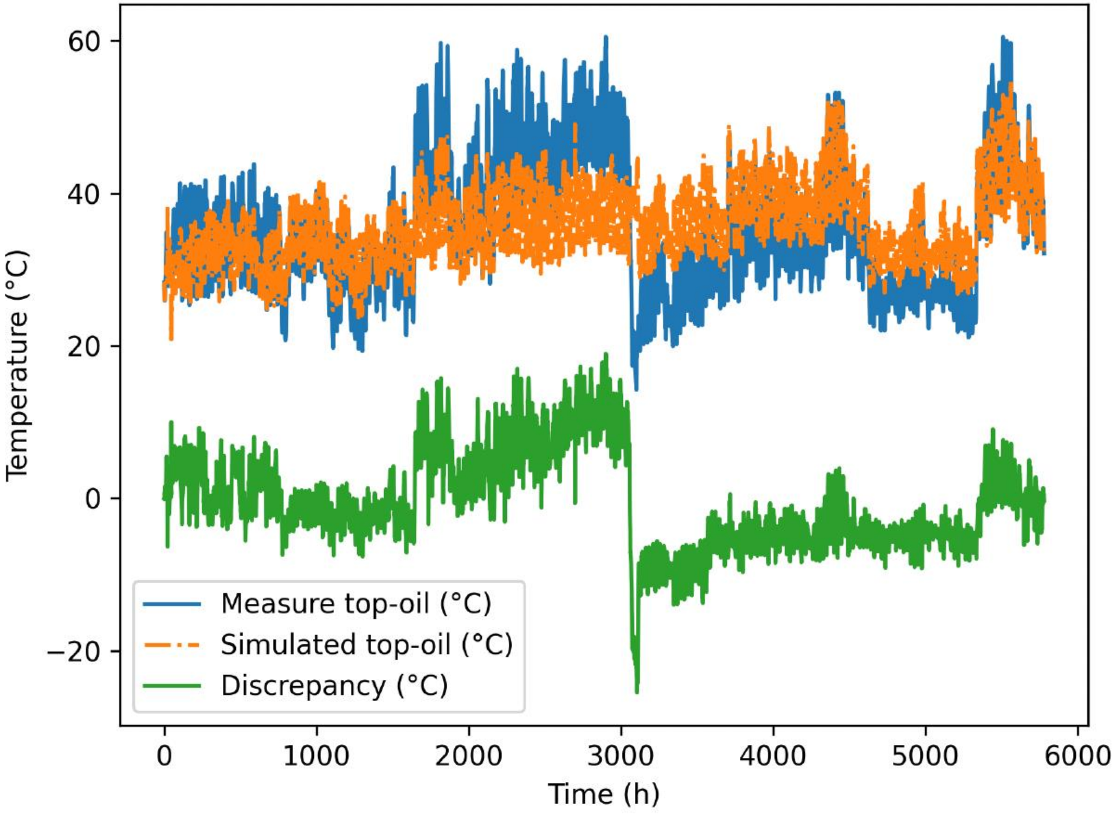




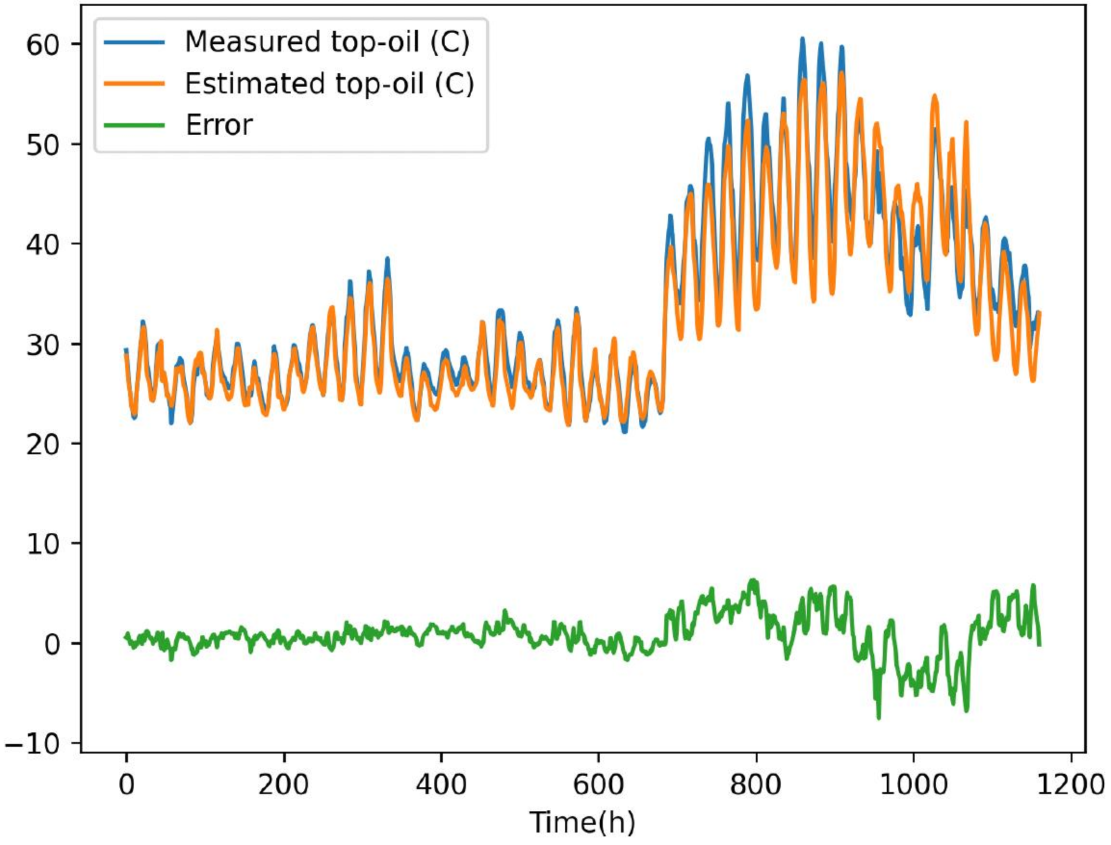
HYBRID

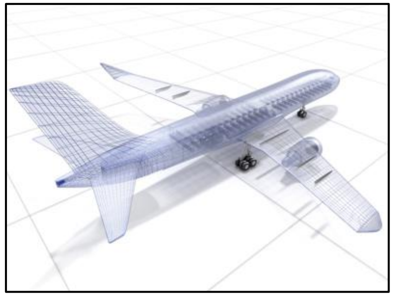


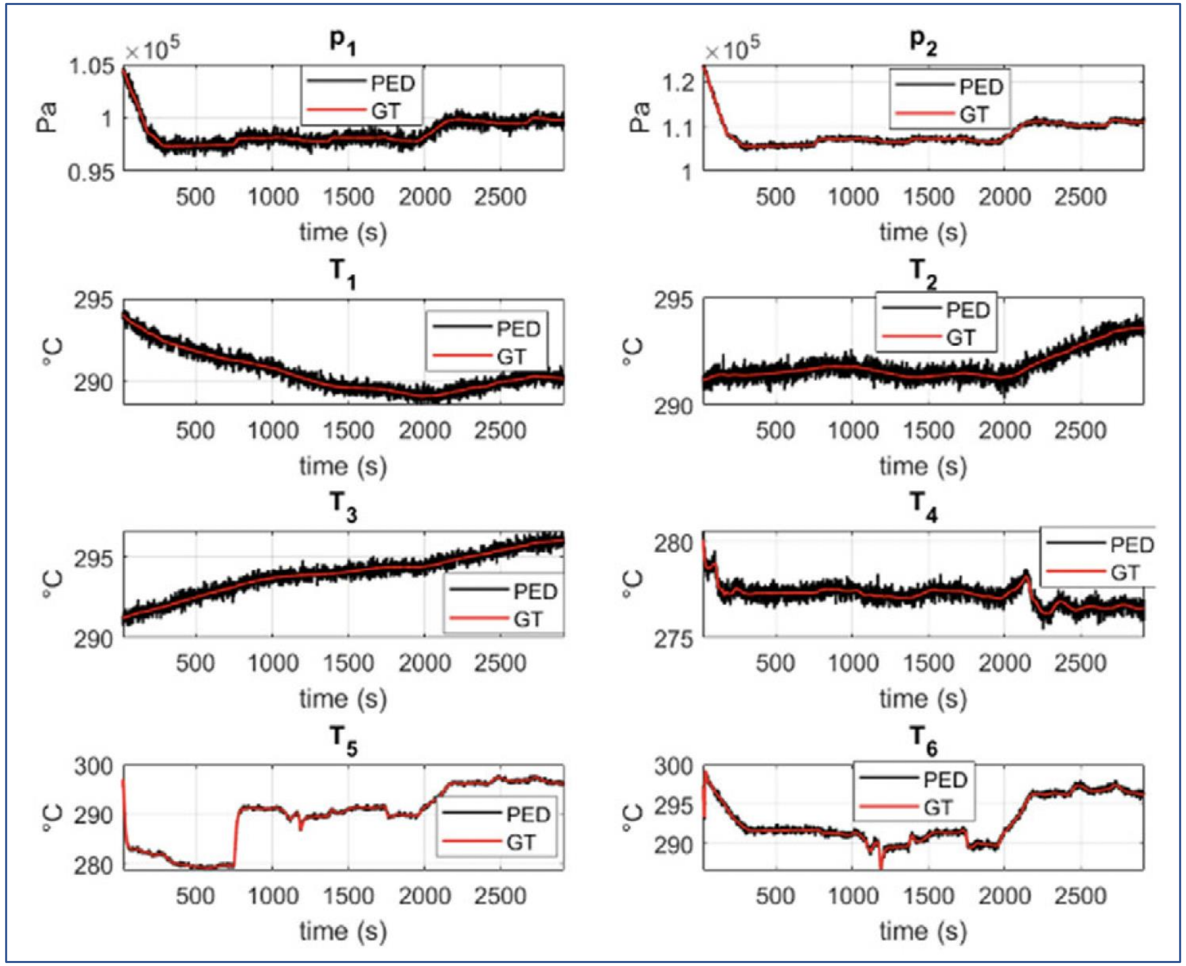
Le réseau
de transport
d'électricité



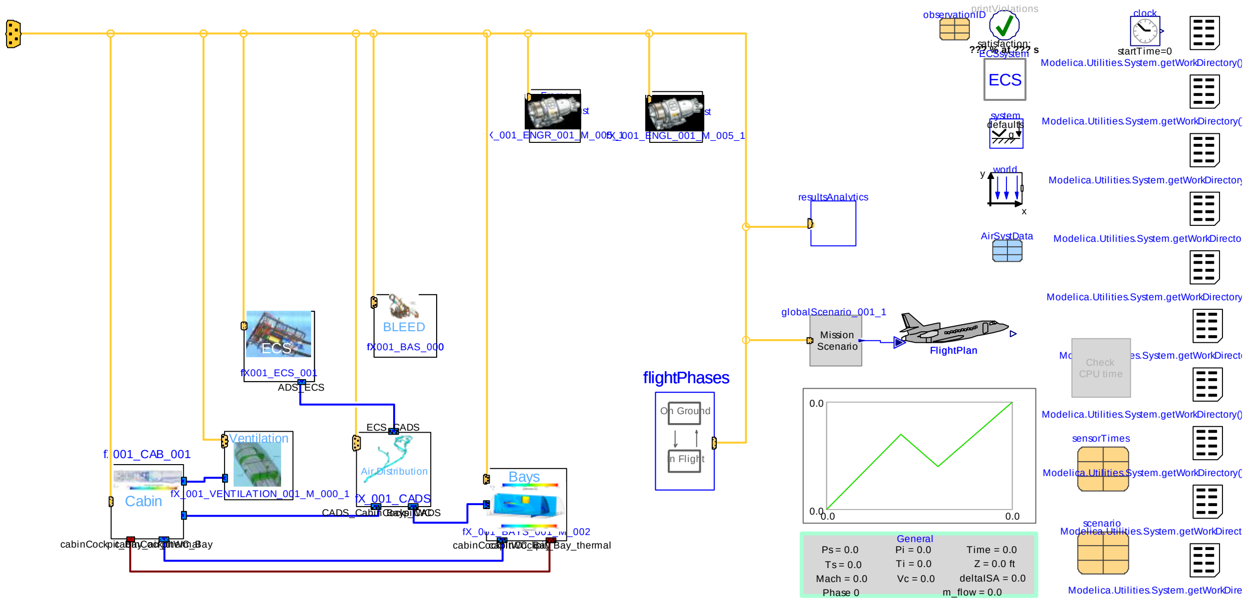
Testing+integration: HT Oil temperature estimation for a RTE transformer



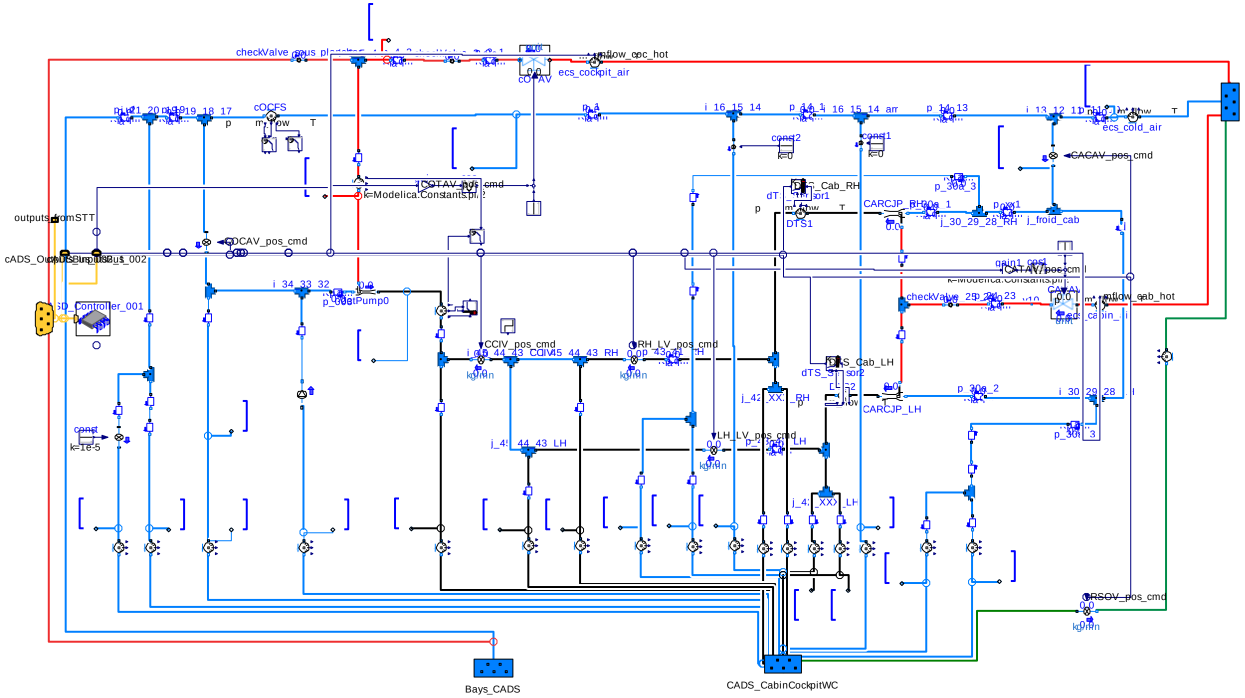




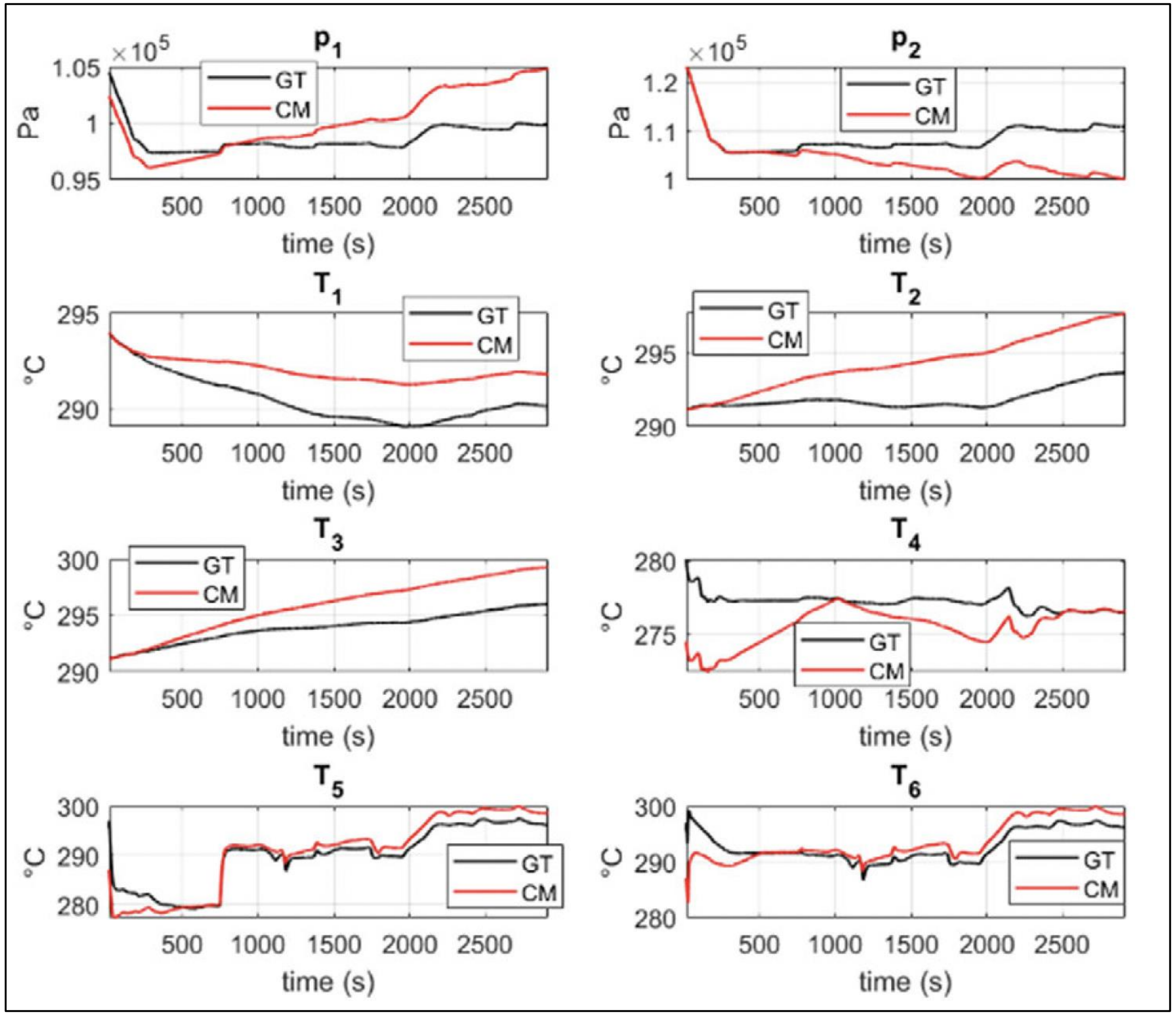
p_1
$\times 10^5$
Pa
PED
GT
time (s)
p_2
T_1
T_2
T_3
T_4
T_5
T_6
°C

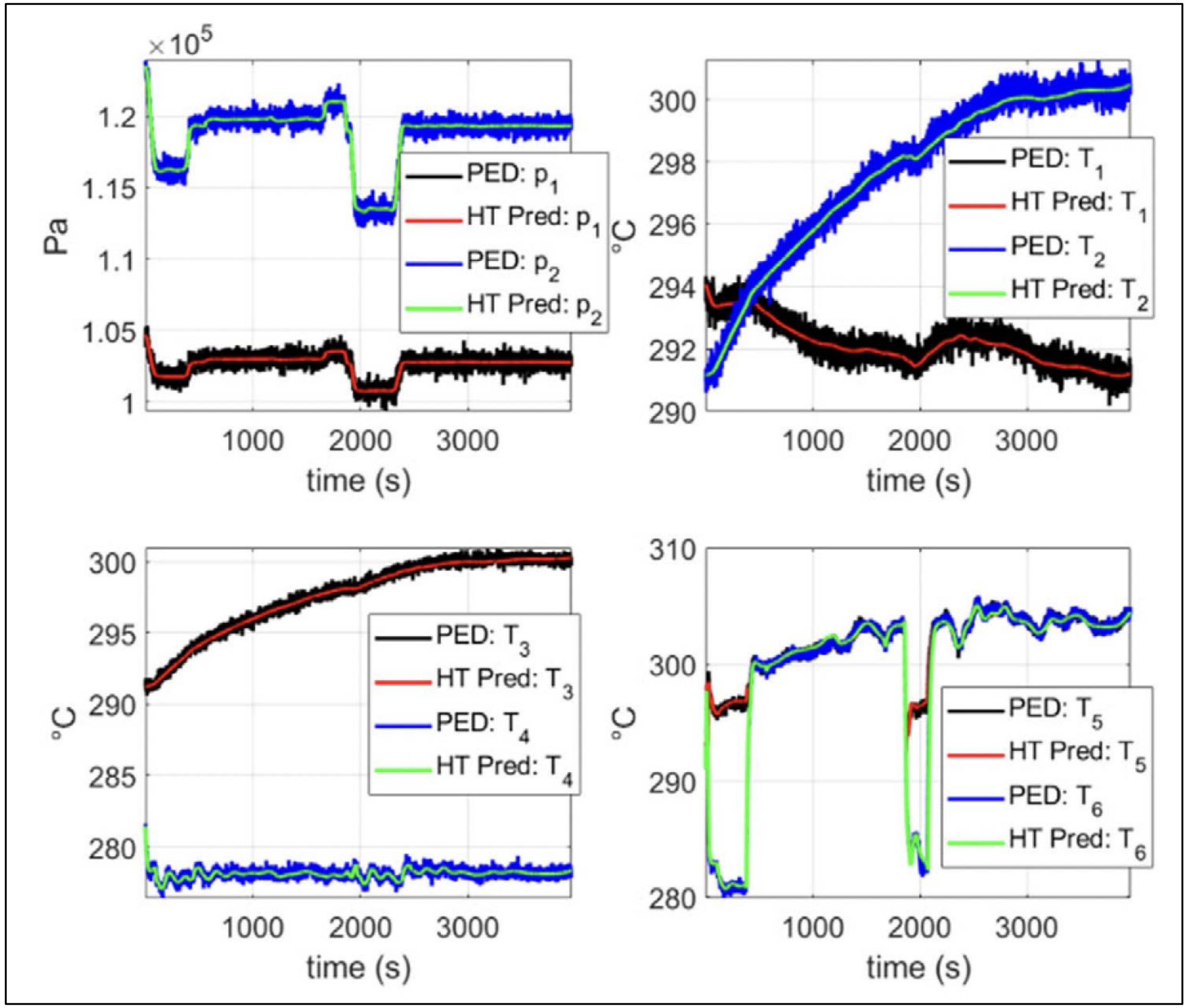


ECS
BLEED
Ventilation
Air Distribution
Cabin
Bays
flightPhases
On Ground
In Flight
Mission Scenario
FlightPlan
resultsAnalytics
globalScenario_001_1
Modelica.Utilities.System.getWorkDirectory()
General
Ps = 0.0
Pi = 0.0
Time = 0.0
Ts = 0.0
Ti = 0.0
Z = 0.0 ft
Mach = 0.0
Vc = 0.0
deltaISA = 0.0
Phase 0
m_flow = 0.0

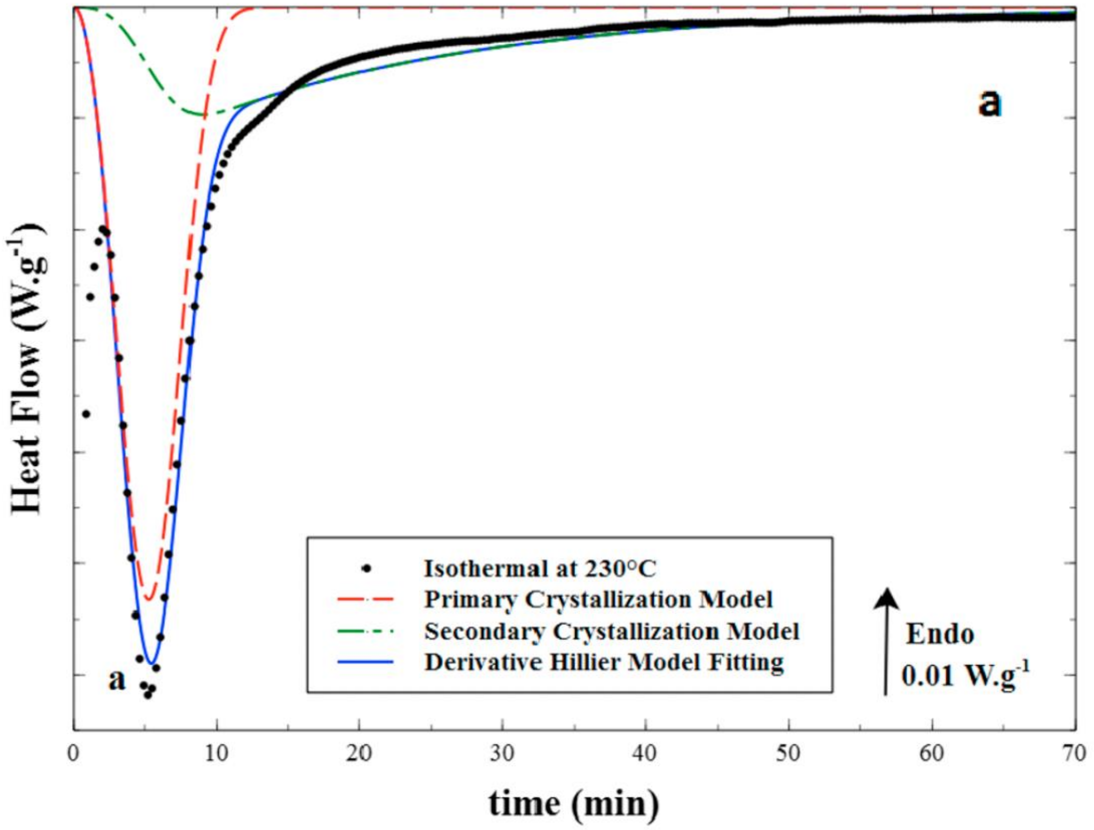


Bays_CADS
CADS_CabinCockpitWC
ecs_cockpit_air
ecs_cold_air


p1
×10^5
GT
CM
Pa
p2
T1
T2
T3
T4
T5
T6
°C
time (s)


×10^5
Pa
PED: p1
HT Pred: p1
PED: p2
HT Pred: p2
PED: T1
HT Pred: T1
PED: T2
HT Pred: T2
PED: T3
HT Pred: T3
PED: T4
HT Pred: T4
PED: T5
HT Pred: T5
PED: T6
HT Pred: T6
°C
time (s)

Hybrid modelling of
local kinetics

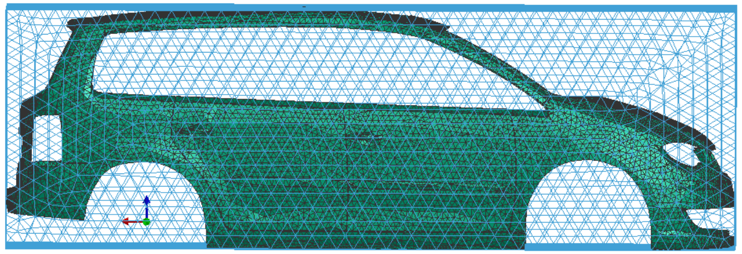


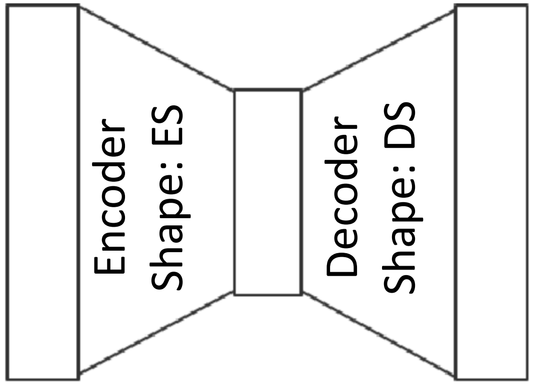
$$\frac{d\alpha}{dt} = f(t;\mathbf{p}) + \mathbf{g}(\mathbf{t};\mathbf{p})$$

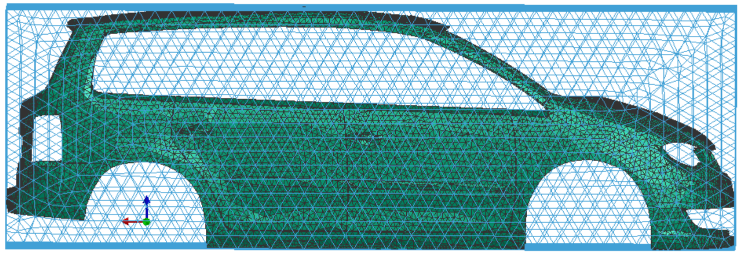
Model

Data-Driven
correction

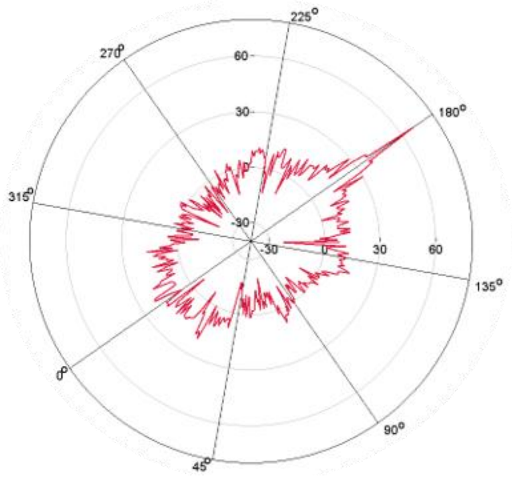
Autoencoder of Shapes: AE-S

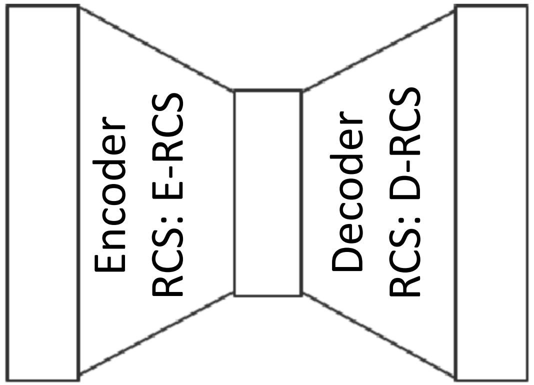


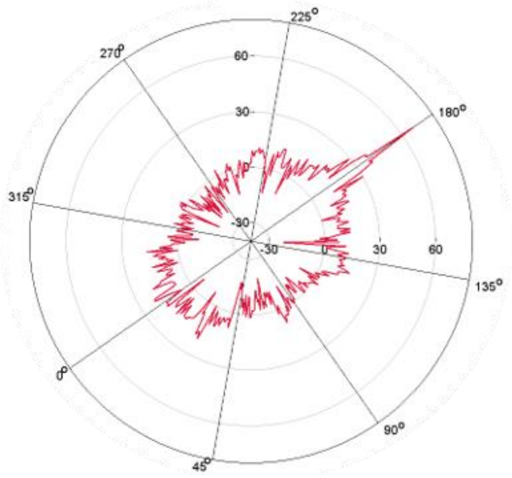


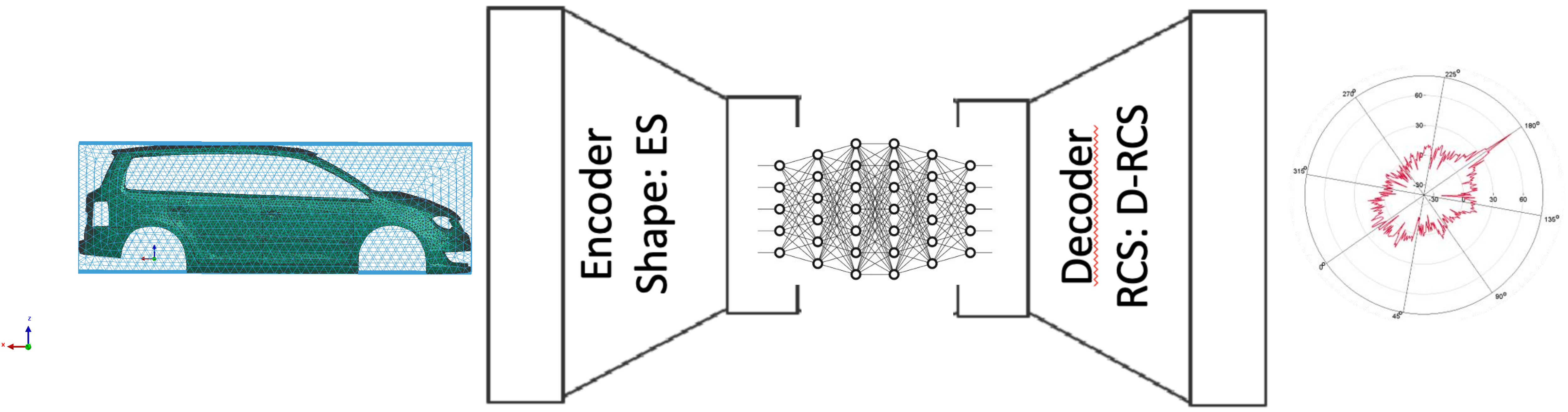


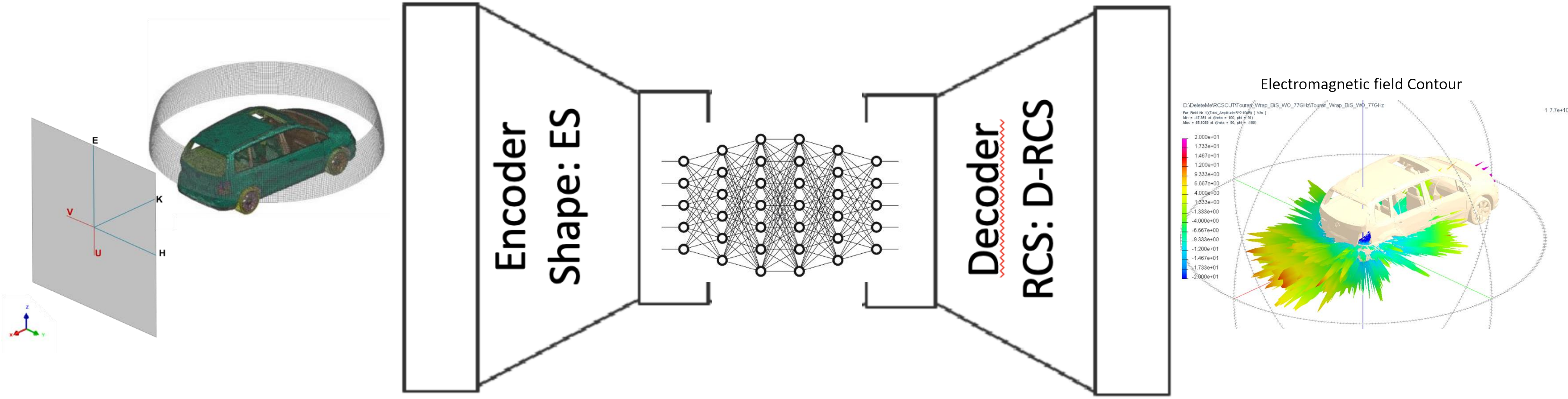
Autoencoder of RCS: AE-RCS



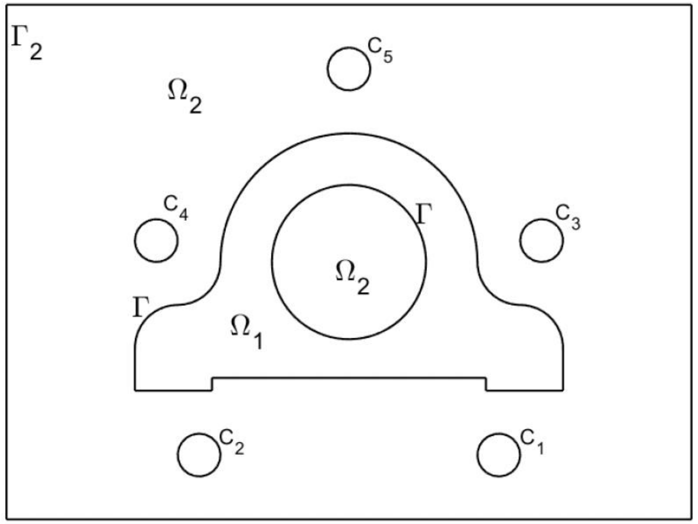


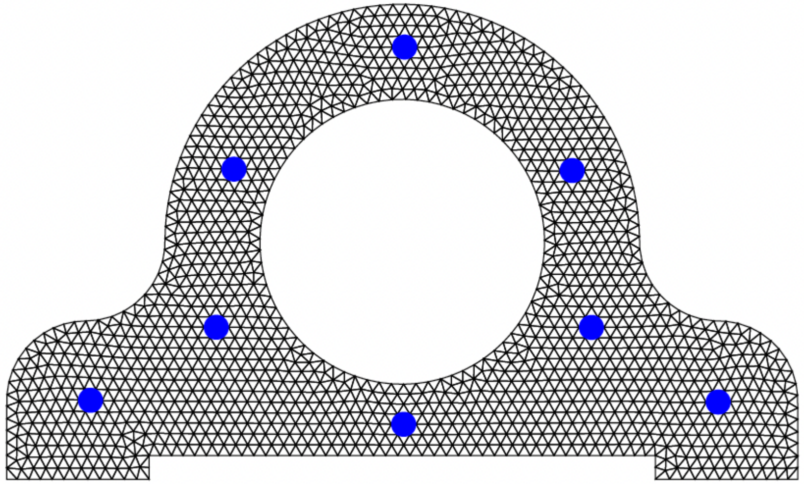


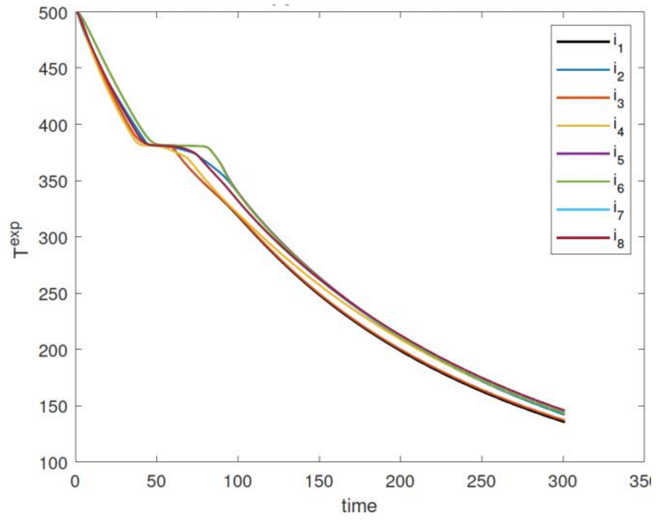

Encoder
Shape: ES
Decoder
RCS: D-RCS

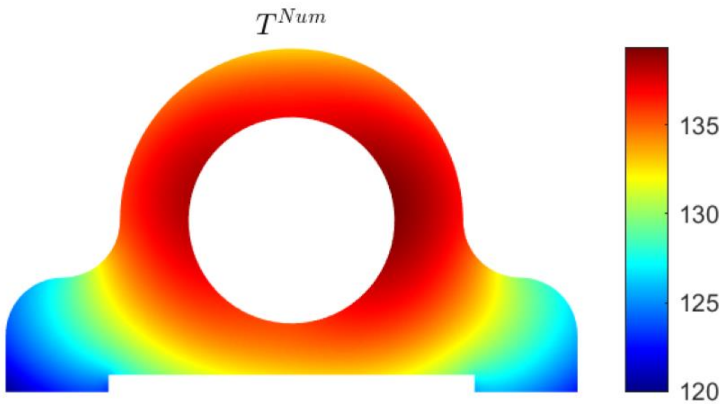

E
K
V
U
H
Encoder
Shape: ES
Decoder
RCS: D-RCS
Electromagnetic field Contour

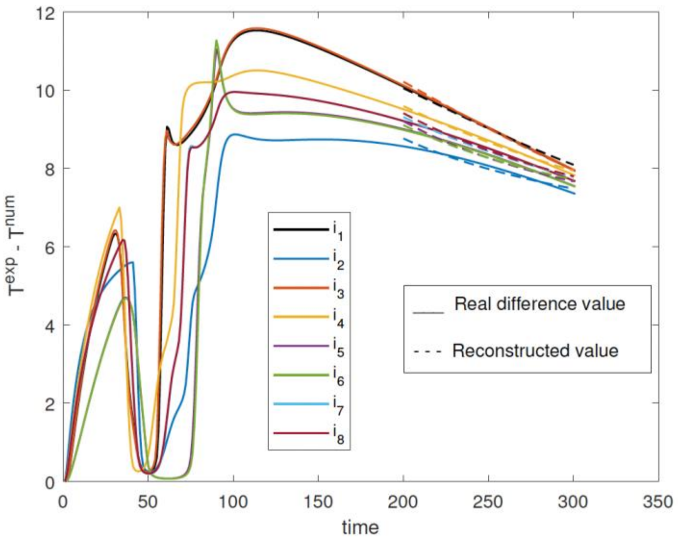
Correcting beyond the observation

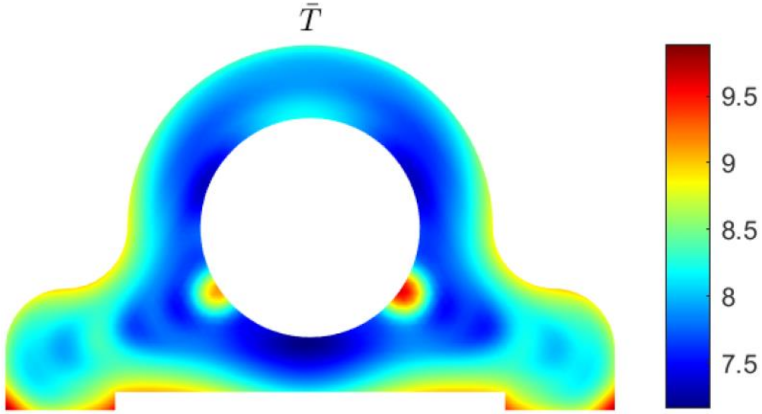


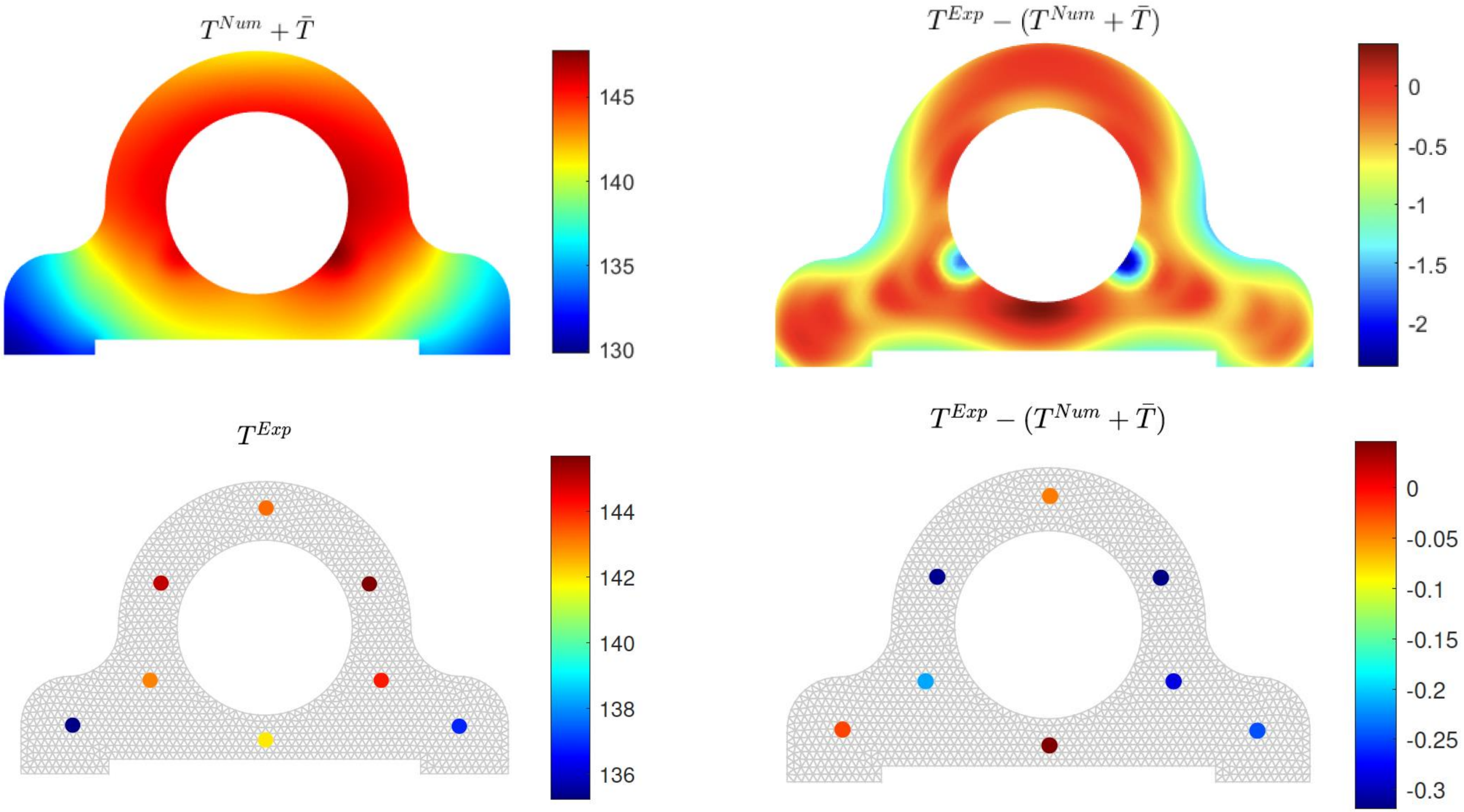











$T^{Num} + \bar{T}$
145
140
135
130
$T^{Exp} - (T^{Num} + \bar{T})$
0
-0.5
-1
-1.5
-2
T^{Exp}
144
142
140
138
136
$T^{Exp} - (T^{Num} + \bar{T})$
0
-0.05
-0.1
-0.15
-0.2
-0.25
-0.3

Cheap simulation + learnt correction

Predicting high-fidelity data from coarse-mesh Computational Fluid Dynamics corrected using Hybrid Twins based on Optimal Transport

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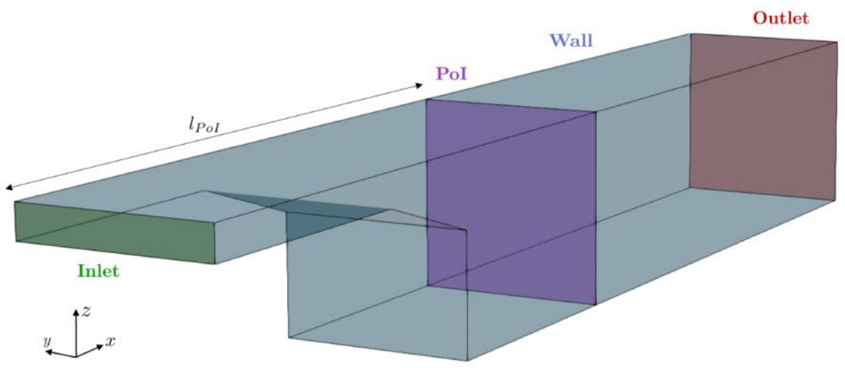
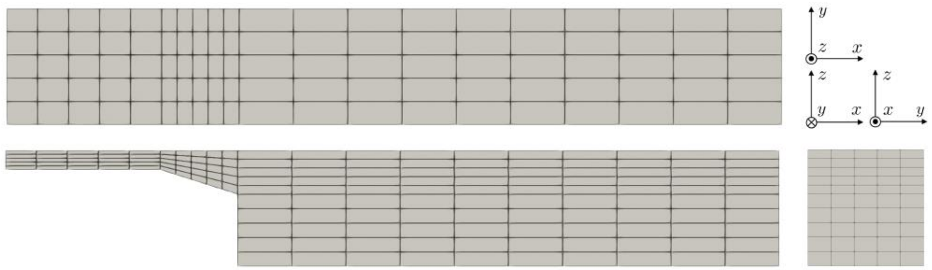
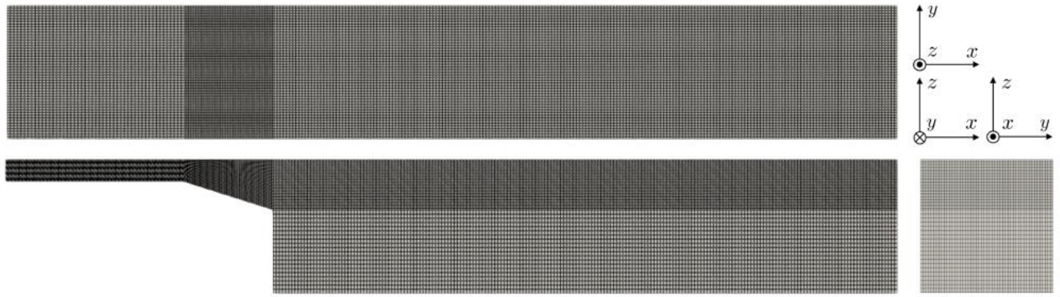
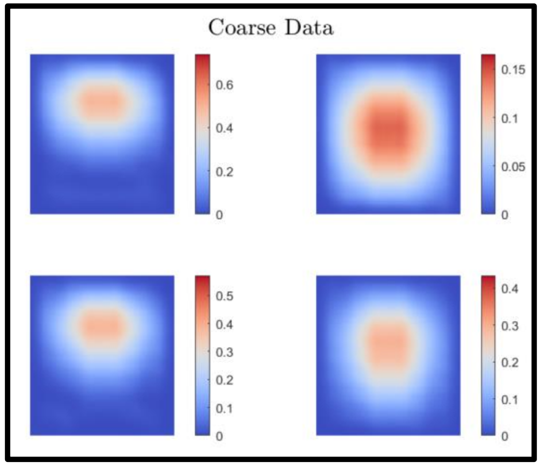
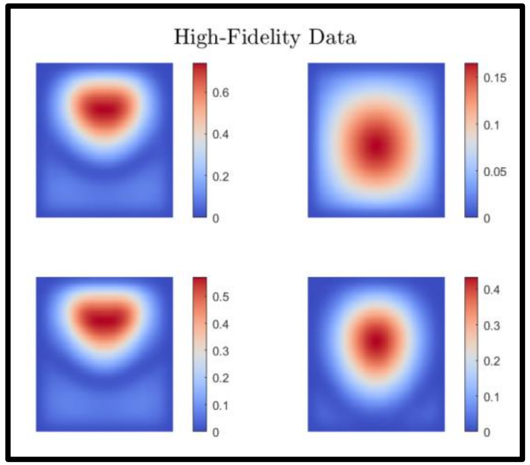




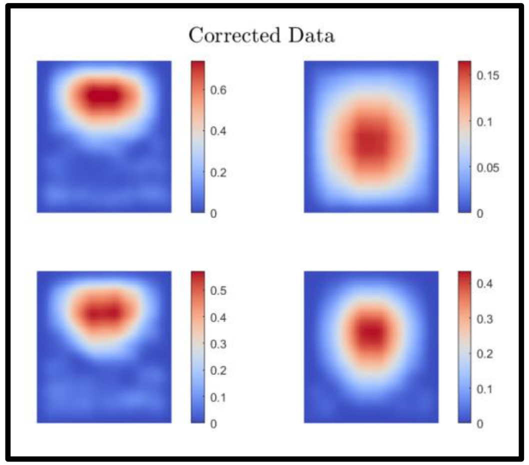




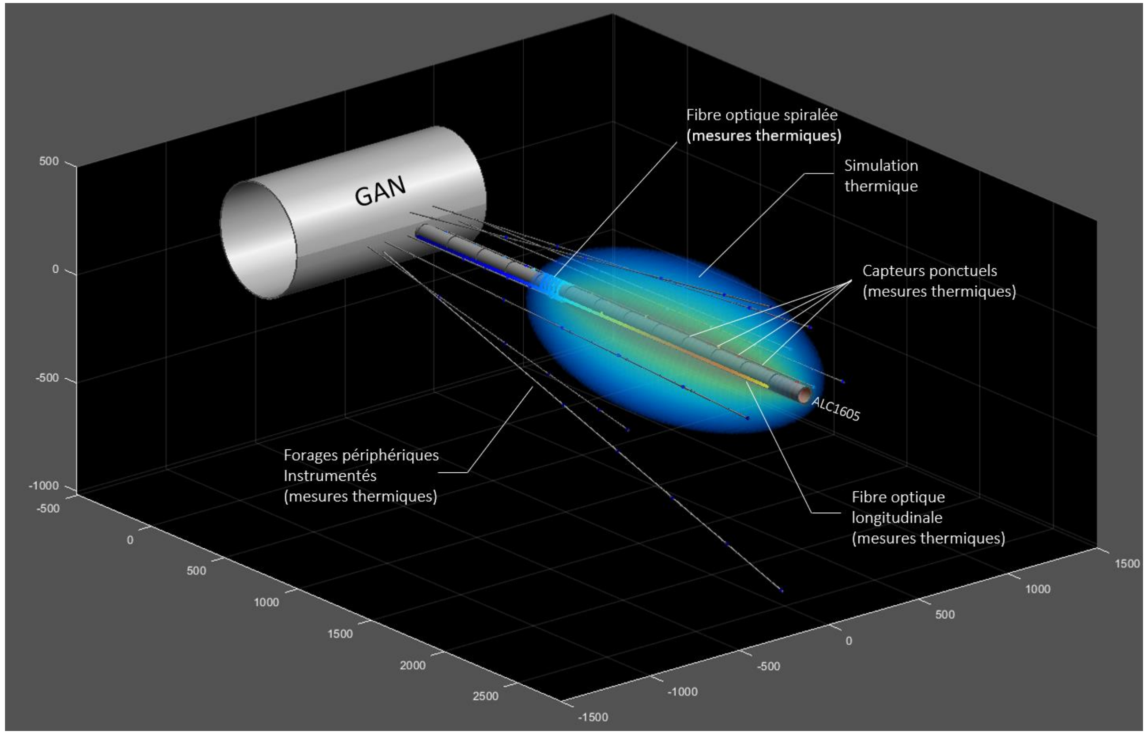


Hamiltonian formalism + QUBO
(quadratic unconstrained binary optimization)
QUANTUM ANEALING

$$\sum_{i,j,k,l}^{N} \sum_{p,q>p}^{P} X_{ij}^{p} \mathcal{D}(P(X_{ij}^{p}), P(X_{kl}^{q})) X_{kl}^{q}$$



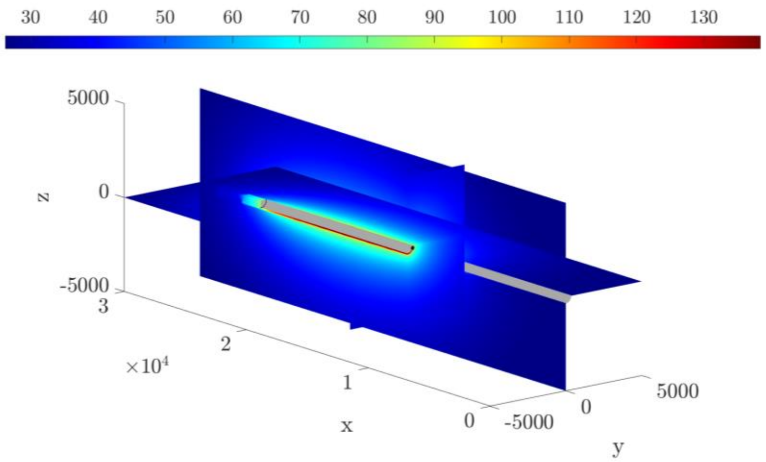
	ε_{max} [%]	ε_{pos} [cm]	W_2^2	$\mathcal{I}$ [%]
Coarse Data	28.5	2.7	0.017	18.7
HT Corrected Data	4.1	1.8	0.007	0.8

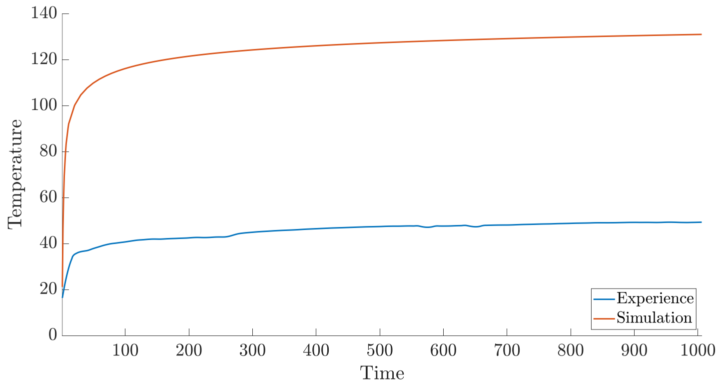


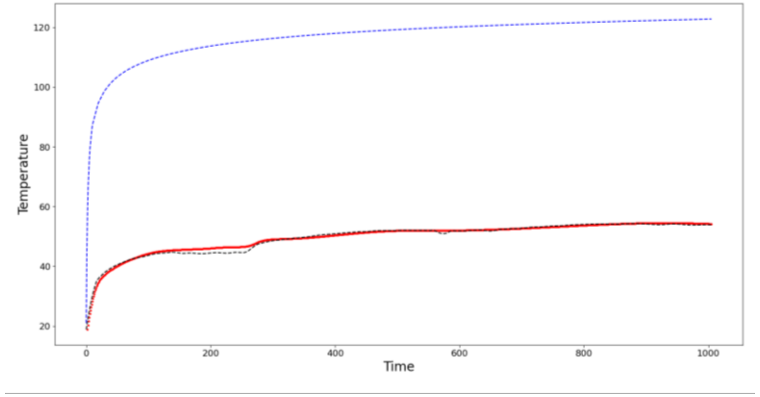
ANDRA
Agence nationale pour la gestion des déchets radioactifs

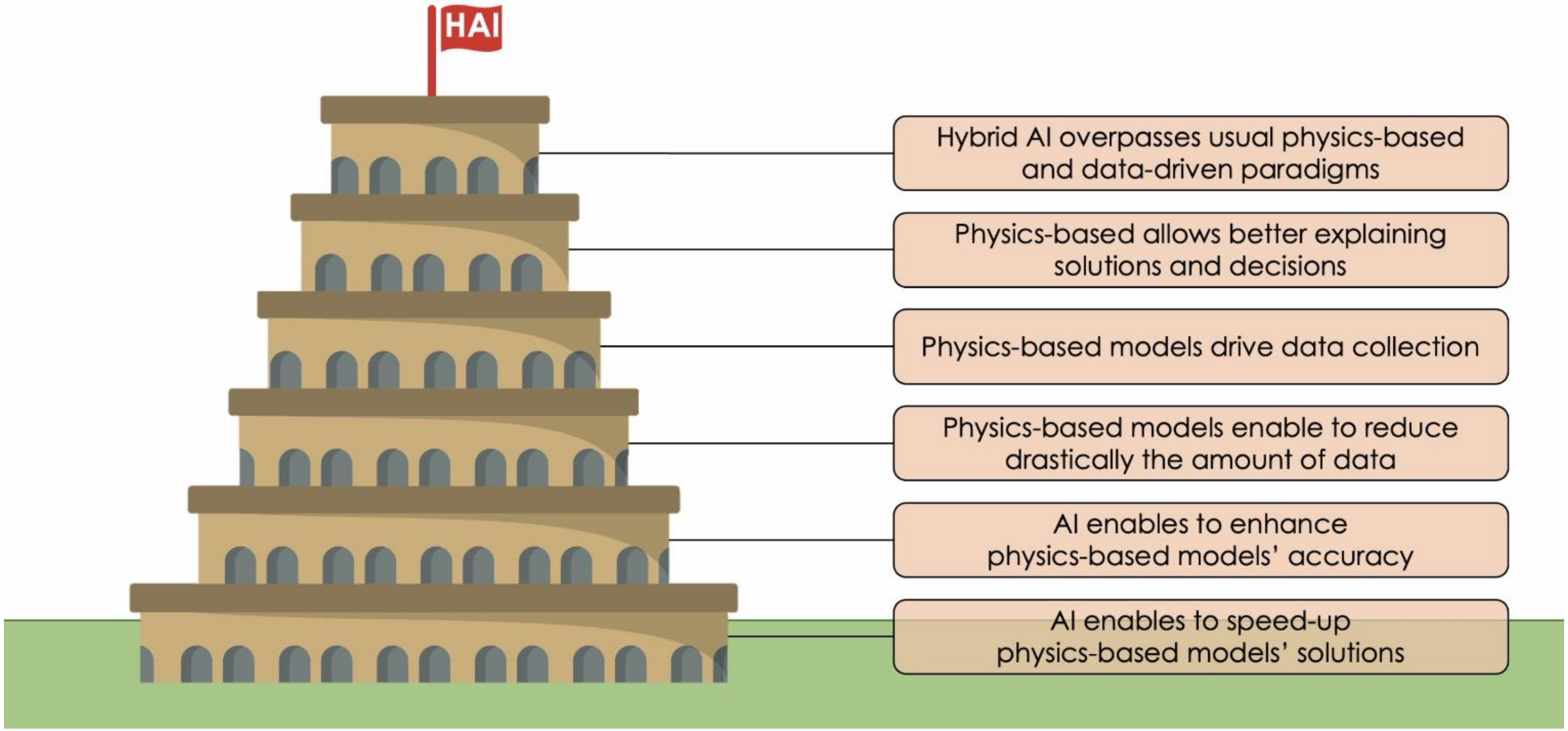
AM VALOR
Arts et Métiers · Sciences et Technologies

esi
get it right








HAI
Hybrid AI overpasses usual physics-based and data-driven paradigms
Physics-based allows better explaining solutions and decisions
Physics-based models drive data collection
Physics-based models enable to reduce drastically the amount of data
AI enables to enhance physics-based models' accuracy
AI enables to speed-up physics-based models' solutions