ADVANCES IN HYBRID MODELING: TOWARDS THE NUMERICAL TRANSITION OF TERRITORIES

Beatriz Moya, Alicia Tierz, Ruben Laurenco, Mariya Gorpinich, Jad Mounayer, Sebastian Rodriguez, Boris Huljak, Sergio Torregrosa, David Gonzalez, Iciar Alfaro, Elias Cueto, Francisco Chinesta

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The hybrid modeling paradigm

Integration of physics-based models and data-driven models to represent, predict, or control a system more accurately, robustly, and efficiently than either approach alone.

In AI....

It is key to avoid hallucinations. Spetially in Generative AI

(Credit: PCMag / Stability AI)

In AI….

It is key to avoid hallucinations. Spetially in Generative AI

(Credit: PCMag / Stability AI)

Objective

Analyzing the role of model order reduction and hybrid modeling for the development of applications towards numerical transition of territories and decision making.

Knowledge-informed generative AI

Hybrid modeling during operation: Singapore (Descartes)

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Knowledge-informed generative AI

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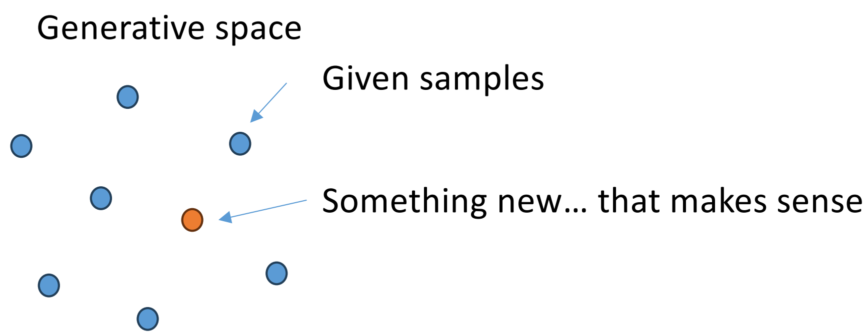
What is generative AI

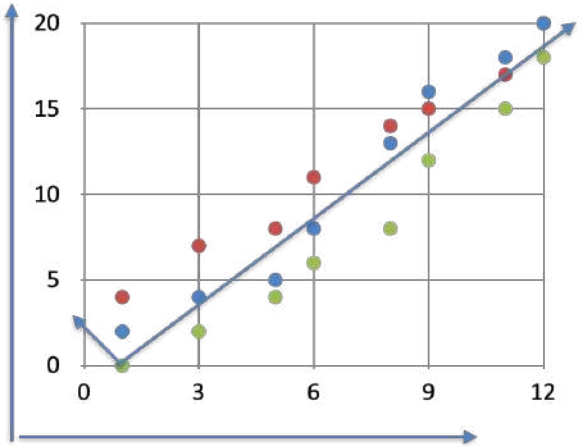
CREATE NEW CONTENT



Gen AI and Model order reduction

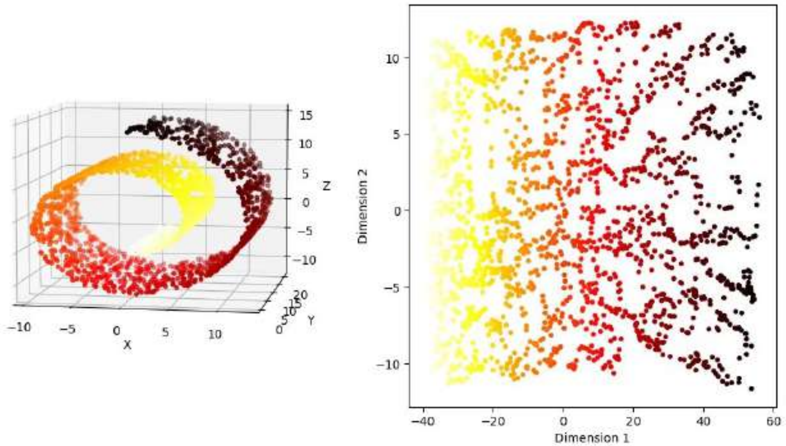
Proper Orthogonal Decomposition

POD



Kernel Principal Component Analysis

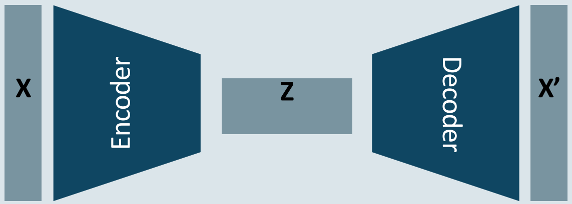
KPCA



No mapping to the original space

Introduction to methods in generative design based on neural networks

Generative design principle : Sampling a latent space **Z** (low-dimensional representation containing all essential features of our data) to generate new data.



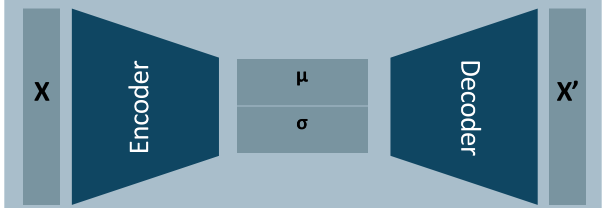
Autoencoders

Pros :

- Easy to train

Cons :

- Potentially irrealistic generated samples



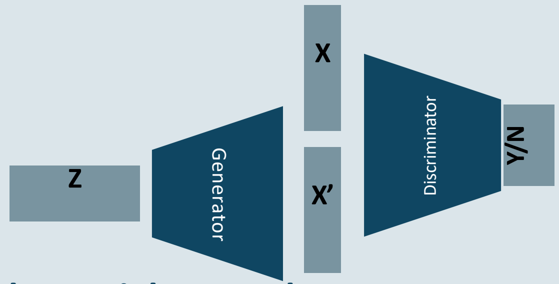
Variational Autoencoders

Pros :

- Realistic generated samples

Cons :

- Low quality samples
- Difficult to train



Adversarial networks

Pros :

- High quality samples

Cons :

- Potentially irrealistic generated samples
- Difficult to train

How to interpolate properly on manifolds to generate new samples

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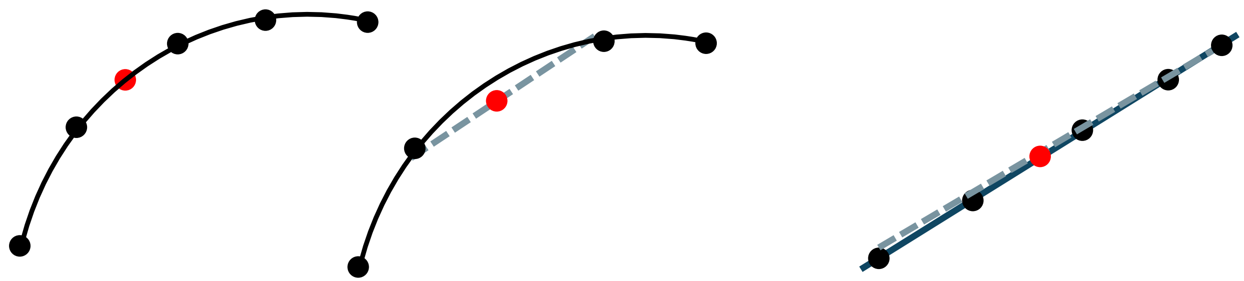
How to interpolate properly on manifolds to generate new samples

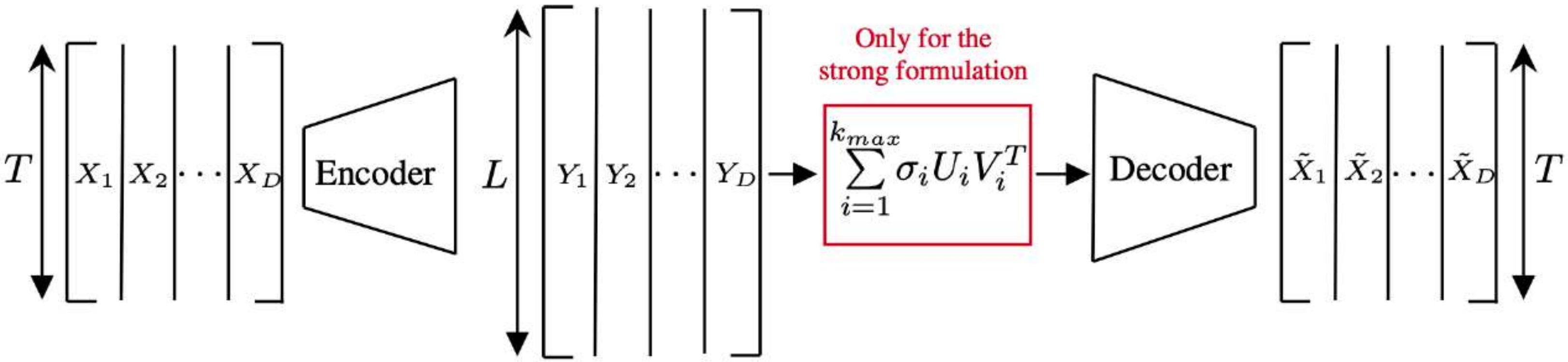


Non-linear interpolation:
What we should do

Linear interpolation:
What we actually do

Linear interpolation:
What we want to do

Rank-reduction autoencoders

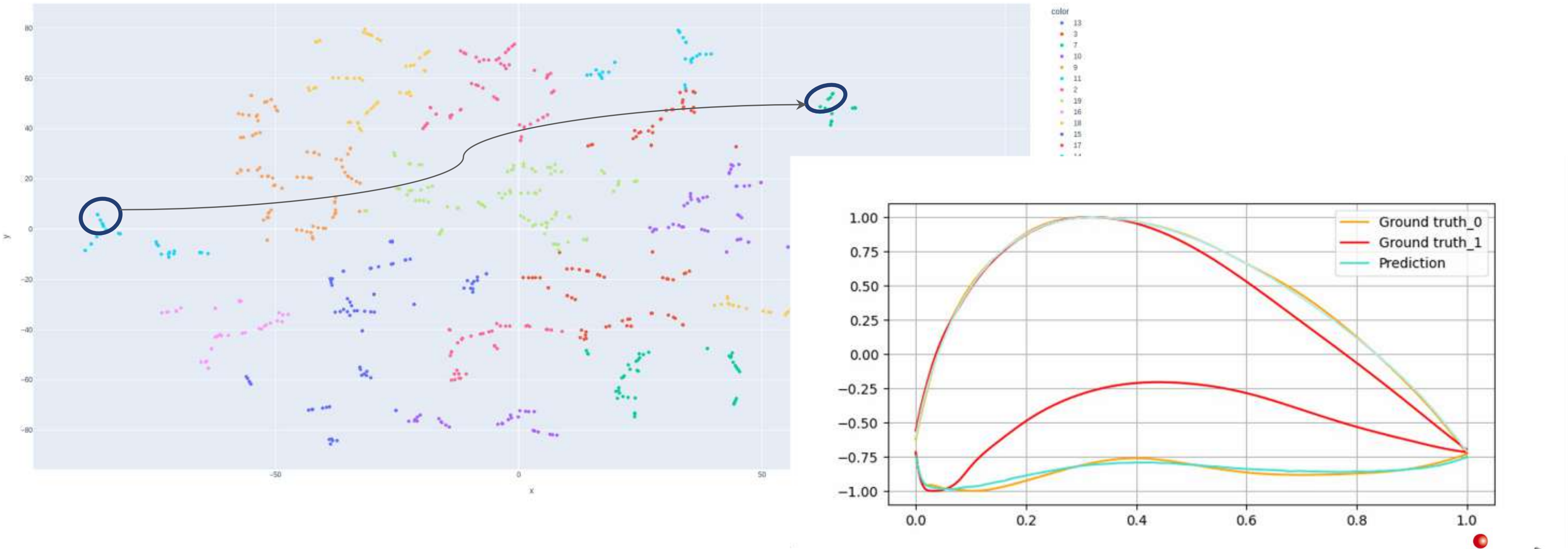


Only for the weak formulation

$$\mathcal{L} = \lambda_1 \| X - \tilde{X} \|_2 \boxed{+ \lambda_2 \| Y - UA \|_2}$$

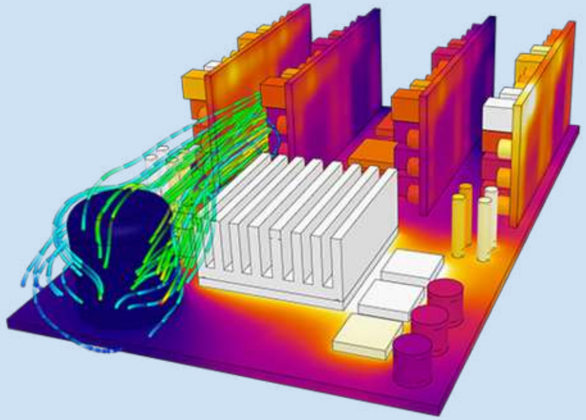
Mounayer, J., Rodriguez, S., Ghnatios, C., Farhat, C., & Chinesta, F. (2024). Rank Reduction Autoencoders--Enhancing interpolation on nonlinear manifolds. *arXiv preprint arXiv:2405.13980*.

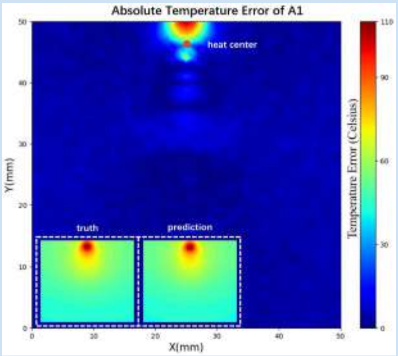
Latent space without “holes”



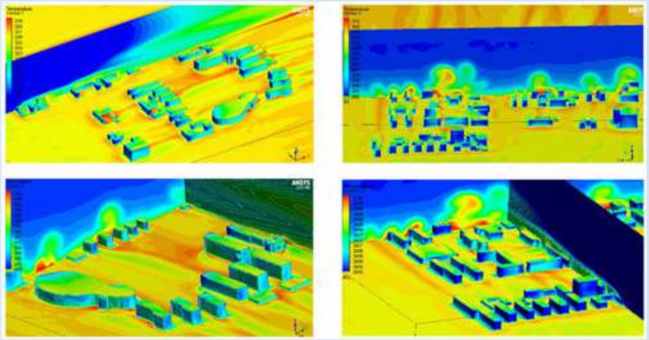
Solvers for resolving temperature fields over complex geometries

Need for parametrization



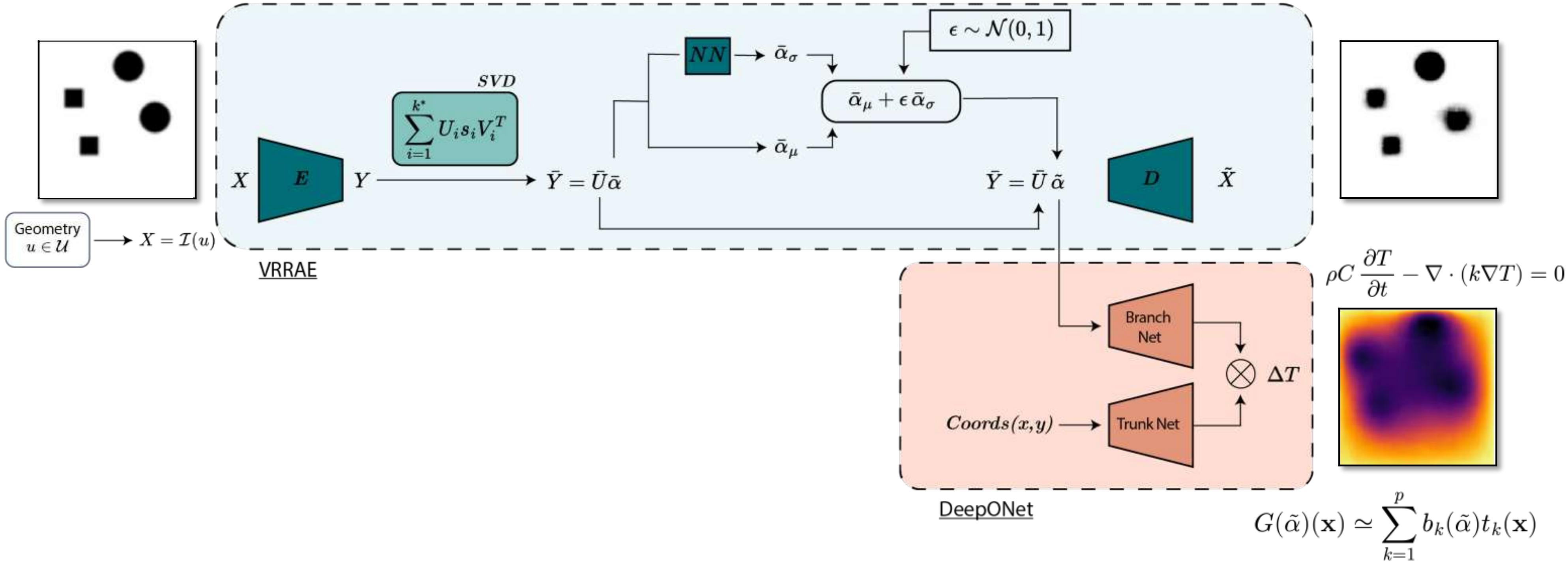


Pan, N. The Temperature Field Prediction and Estimation of Ti-Al Alloy Twin-Wire Plasma Arc Additive Manufacturing Using a One-Dimensional Convolution Neural Networ



Huo, H.; Chen, F. A Study of Simulation of the Urban Space 3D Temperature Field at a Community Scale Based on High-Resolution Remote Sensing and CFD.

Proposed hybrid framework: VRRAE + DeepONet



Four geometries dataset:

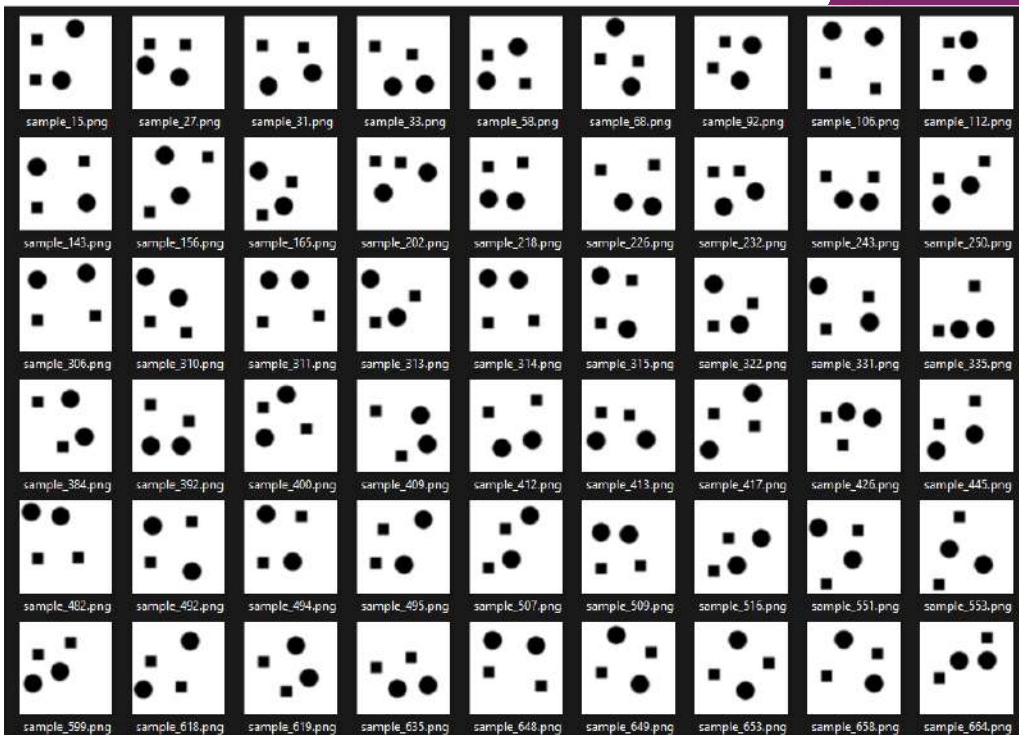
2 Circles, 2 Squares

variables:

4 x position

4 y position

Flag square/circle



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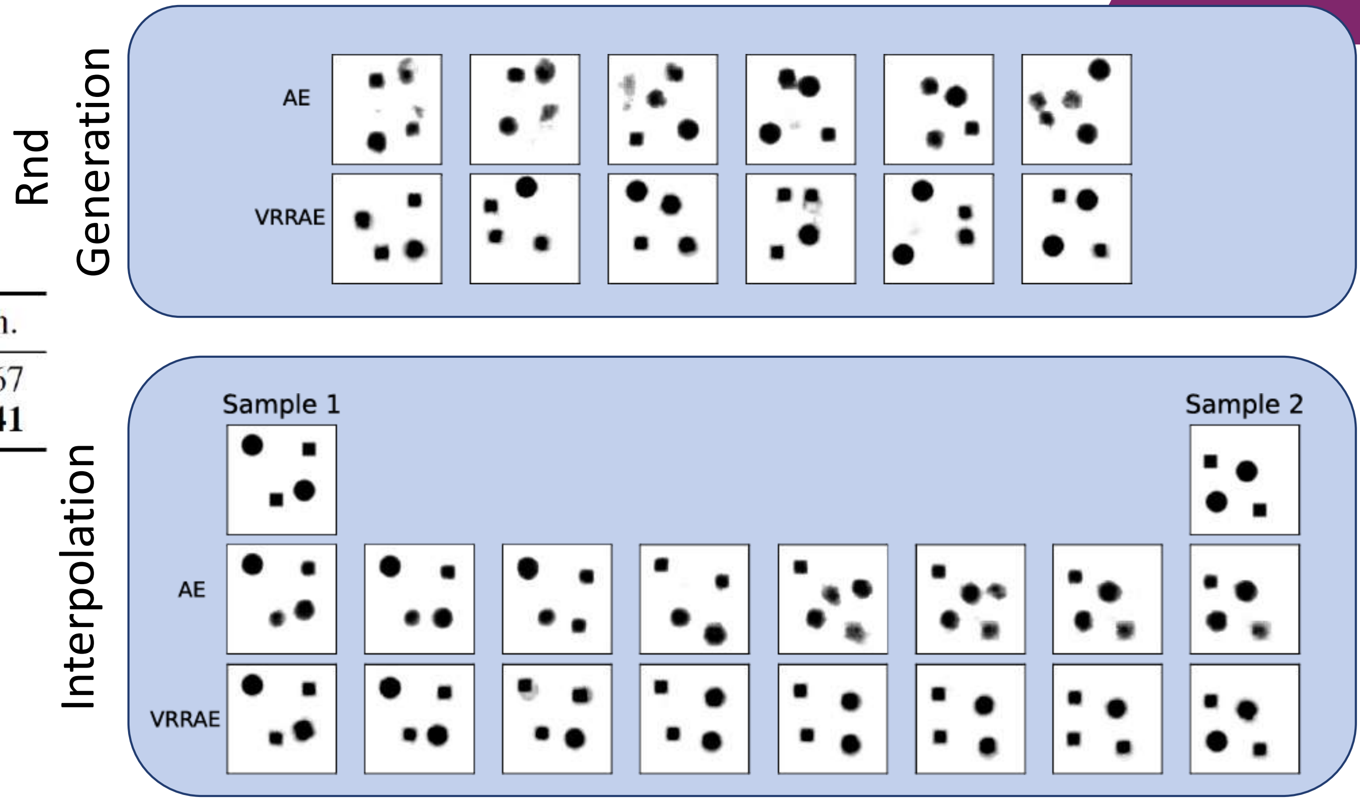
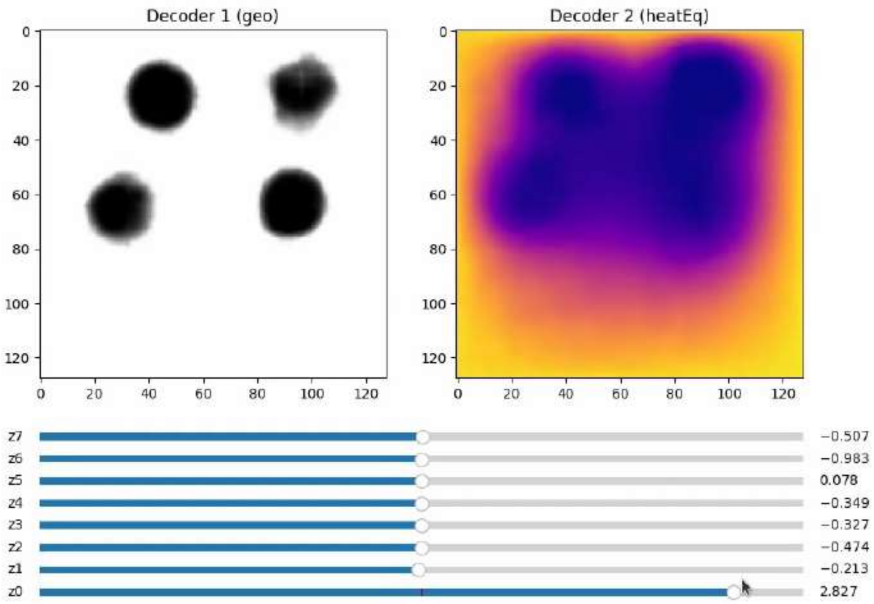
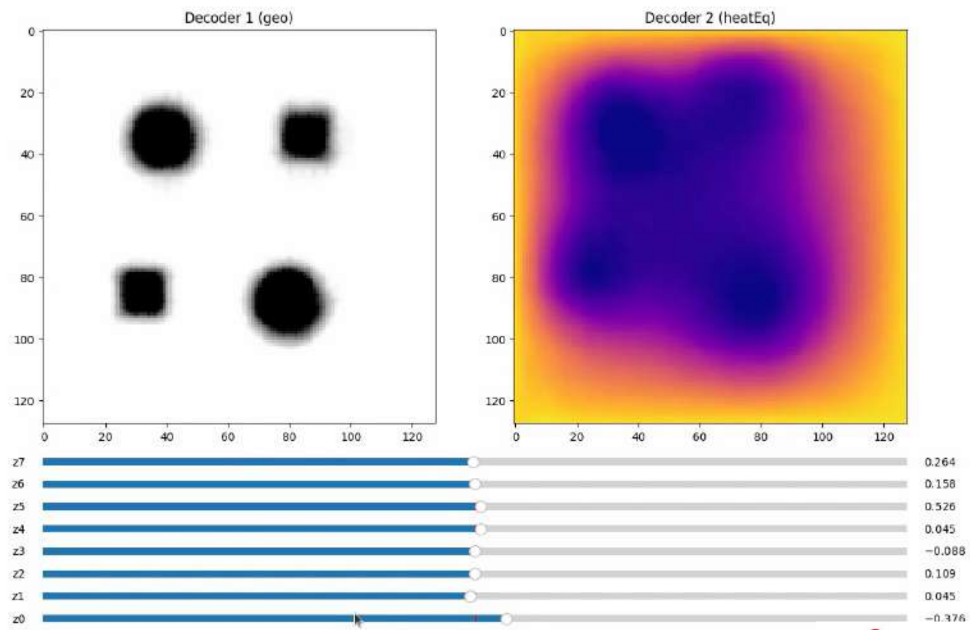
Latent space with K_max=8

Model	Mean MSE	Inter.	Rdn.
AE	0.00892	0.714	0.567
VRRAE	**0.00820**	**0.868**	**0.741**



Results combine two architecures





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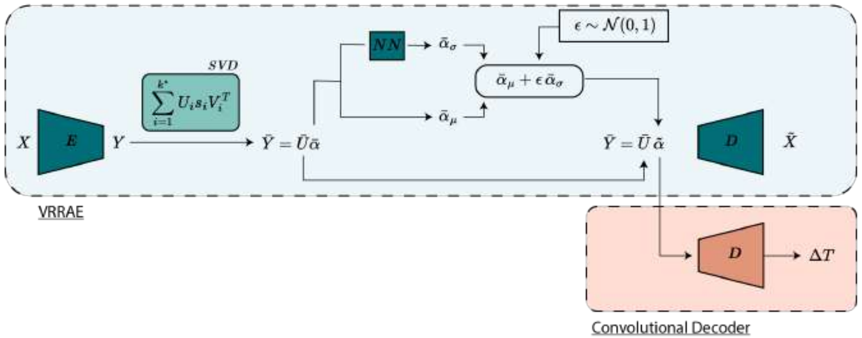
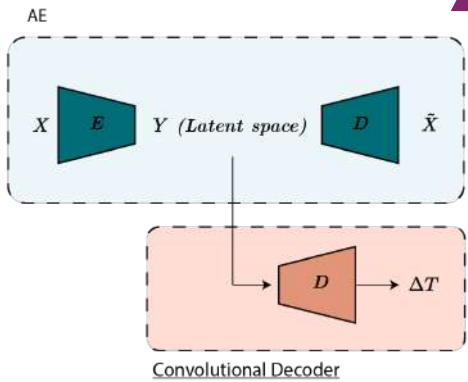
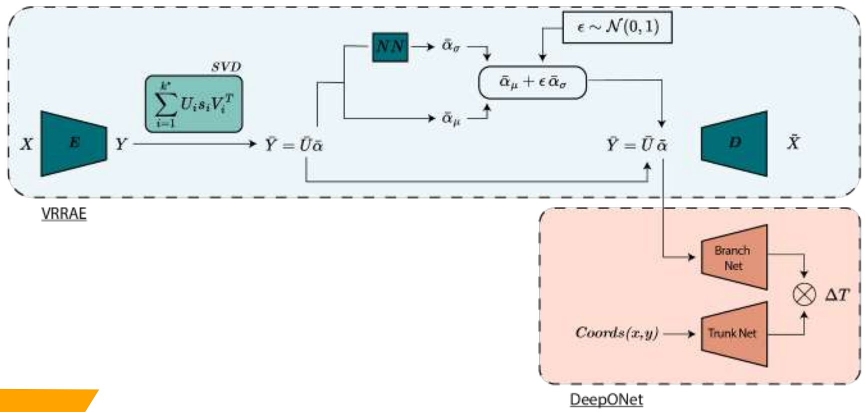
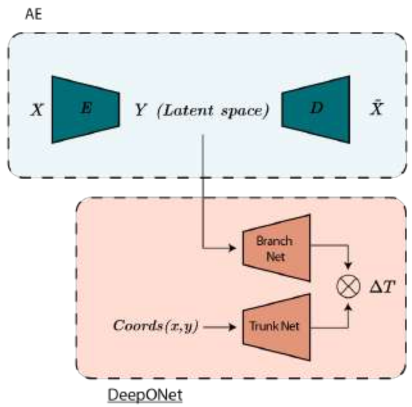
2×2 Component Analysis









Results

2×2 Component Analysis: Encoder (AE vs VRRAE) × Head (CNN vs DeepONet)

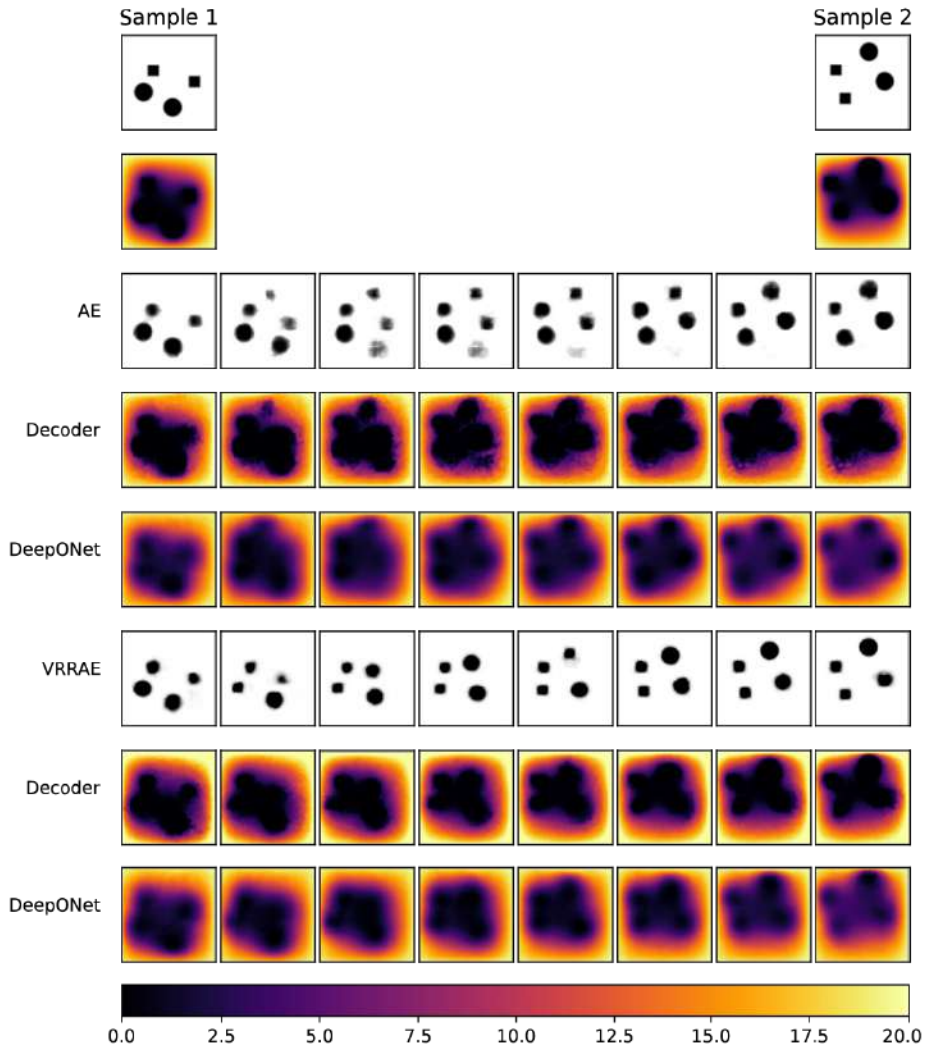
Model	MSE	NMSE	inf_nrm
AE+CNN	$(5.22 \pm 4.85) \times 10^{-3}$	$(9.30 \pm 8.76) \times 10^{-7}$	0.1150 ± 0.0447
AE+DeepONet	$(3.95 \pm 1.63) \times 10^{-3}$	$(7.03 \pm 2.82) \times 10^{-7}$	0.1060 ± 0.0168
VRRAE+CNN	$(3.17 \pm 3.38) \times 10^{-3}$	$(5.68 \pm 6.59) \times 10^{-7}$	$\mathbf{0.0896 \pm 0.0357}$
VRRAE+DeepONet	$\mathbf{(3.12 \pm 1.16) \times 10^{-3}}$	$\mathbf{(5.54 \pm 2.02) \times 10^{-7}}$	0.0942 ± 0.0138

VRRAE+DeepONet = best accuracy + stability

Computational Efficiency

- Matlab (FEM solver): ~0.27 s per sample
- DeepONet: ~0.0026 s per sample

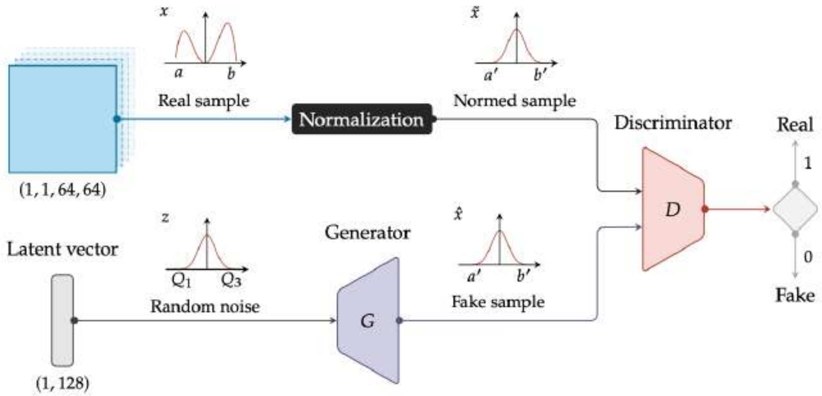
Results

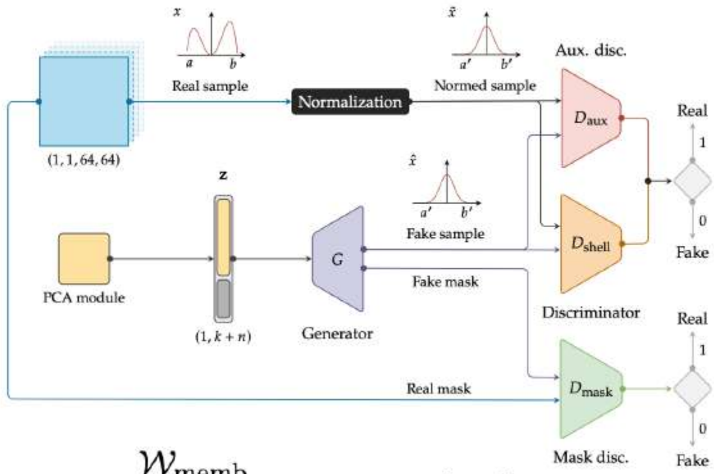


Sample 1
Sample 2
AE
Decoder
DeepONet
VRRAE
Decoder
DeepONet
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0

How to avoid mode collapse

How to avoid mode collapse

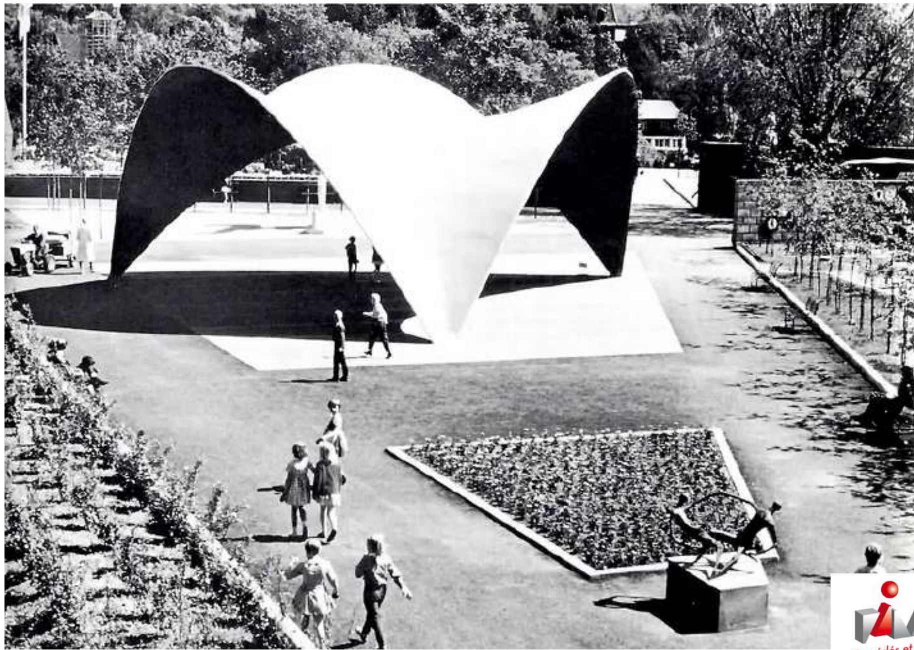




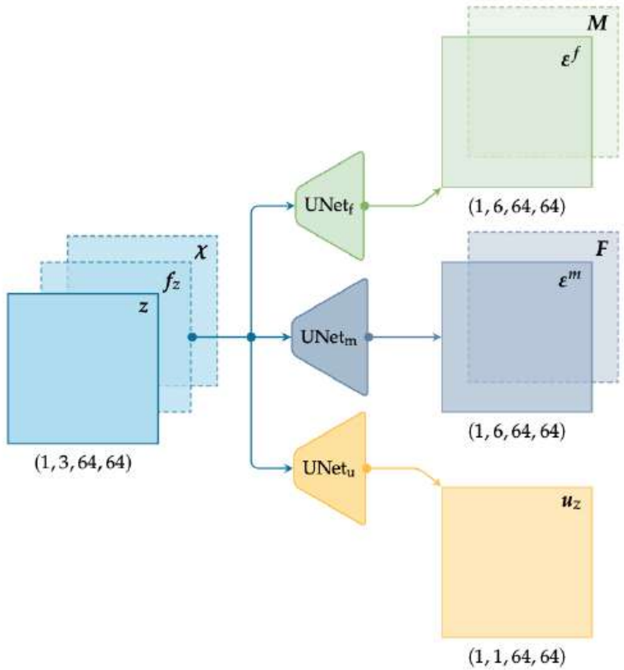
$$m_f = \frac{\mathcal{W}_{\text{memb}}}{\mathcal{W}_{\text{memb}} + \mathcal{W}_{\text{flex}}}, \quad m_f \in [0, 1]$$

$$\mathcal{L}_{G_{\text{total}}} = \mathcal{L}^{\text{fake}}_{G_{\text{shell}}} + \mathcal{L}^{\text{fake}}_{G_{\text{mask}}} + \mathcal{L}_{\text{FM}} + \lambda_{D_{\text{aux}}} \cdot \mathcal{L}^{\text{fake}}_{D_{\text{aux}}}$$

Shell structures



Physics-informed discriminator



$$\mathcal{W}_{\text{memb}} = \int_\Gamma F_{11}\varepsilon^m_{11} + F_{22}\varepsilon^m_{22} + F_{12}\gamma^m_{12} \; d\xi_1 d\xi_2,$$

$$\mathcal{W}_{\text{flex}} = \int_\Gamma M_{11}\varepsilon^f_{11} + M_{22}\varepsilon^f_{22} + M_{12}\gamma^f_{12} \; d\xi_1 d\xi_2,$$

$$\mathcal{W}_{\text{ext}} = \int_\Gamma \boldsymbol{f}^\top_{\text{ext}} \cdot \boldsymbol{u} \; d\xi_1 d\xi_2,$$

$$\delta\mathcal{P} = \mathcal{W}_{\text{memb}} + \mathcal{W}_{\text{flex}} - \mathcal{W}_{\text{ext}} = 0;$$

$$\mathcal{L}_{\text{PB-PUNet}} = \|\boldsymbol{y} - \hat{\boldsymbol{y}}\|_2^2 + \lambda_{\text{phys}} \cdot \delta\mathcal{P}(\hat{\boldsymbol{y}});$$

$$m_f = \frac{\mathcal{W}_{\text{memb}}}{\mathcal{W}_{\text{memb}} + \mathcal{W}_{\text{flex}}}, \quad m_f \in [0, 1]$$

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Bastek, J. H., & Kochmann, D. M. (2023). Physics-informed neural networks for shell structures. *European Journal of Mechanics-A/Solids*, *97*, 104849.

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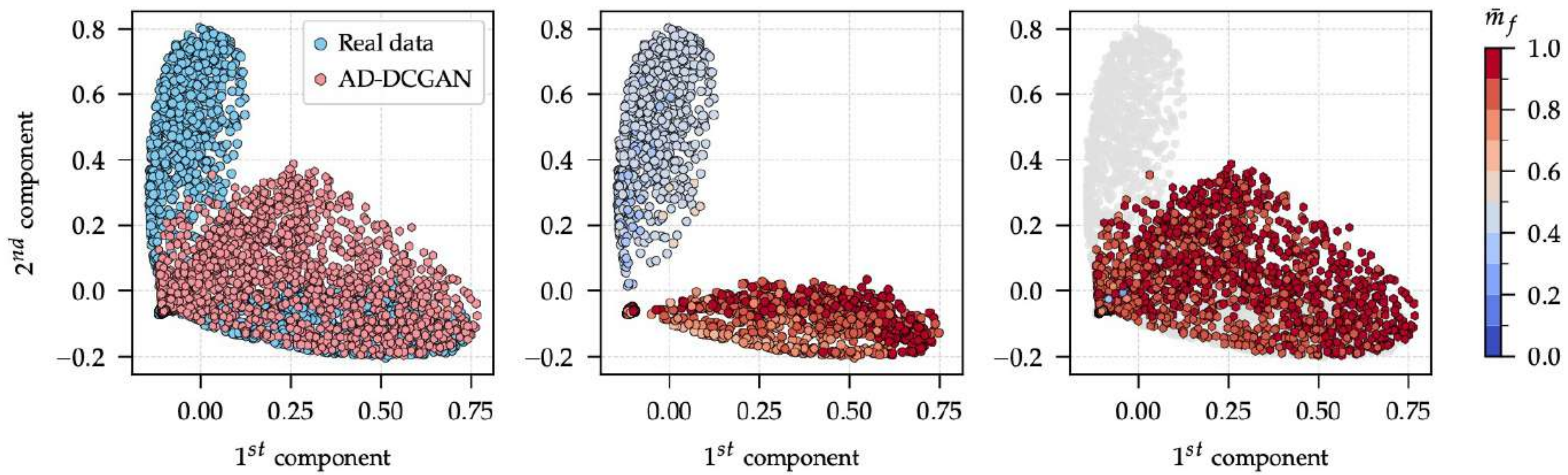
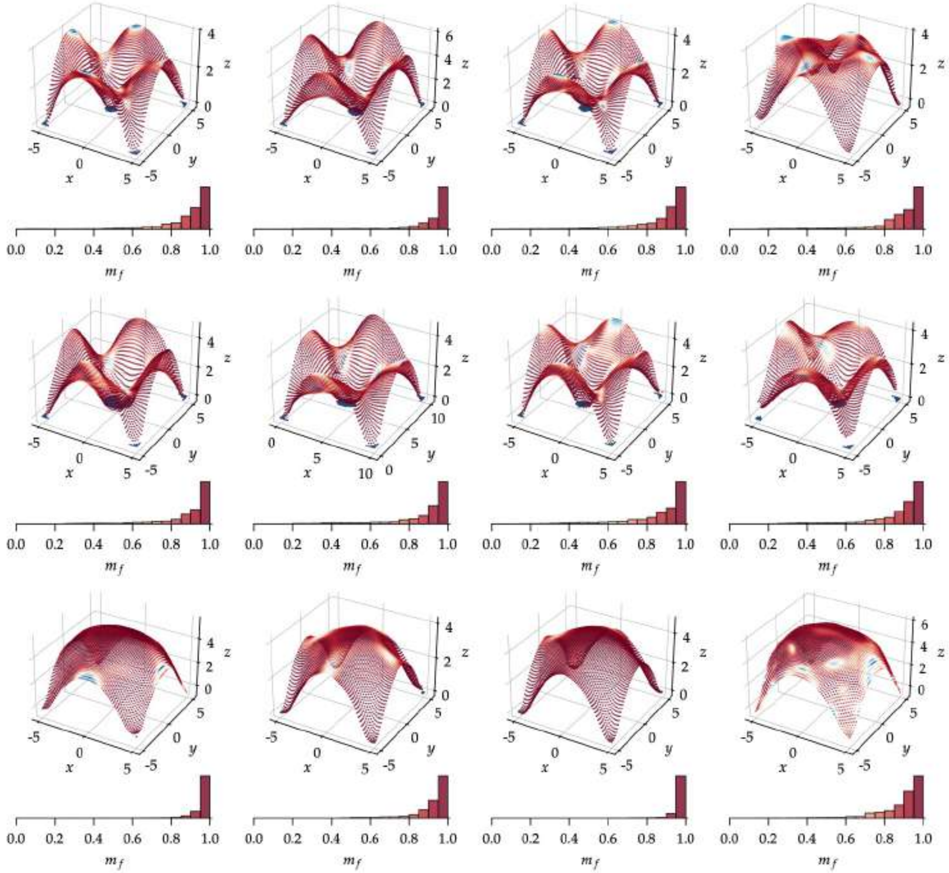
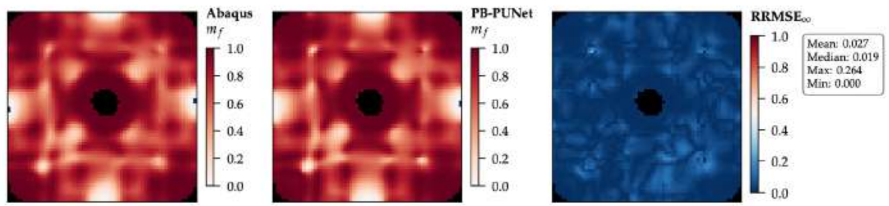
Filling in the manifold







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Hybrid modeling during operation: Singapore (Descartes)

DesCartes

Key Cumulative Figures

$25M

GRANT FROM NRF (SGD)

$5M

PHDs GRANT FROM NTU, NUS, A*STAR & CNRS (SGD)

4

COLLABORATION PROJECTS WITH LOCAL AGENCIES

23

ACADEMIC MEMBERS

11

INDUSTRIAL PARTNERS

5 YEARS

OCT 2021 – OCT 2026

204

RESEARCHERS

INCLUDING:
80 PIs
94 RA & RF
30 PhD Students

SG ECOSYSTEM

230

PAPERS PUBLISHED

3

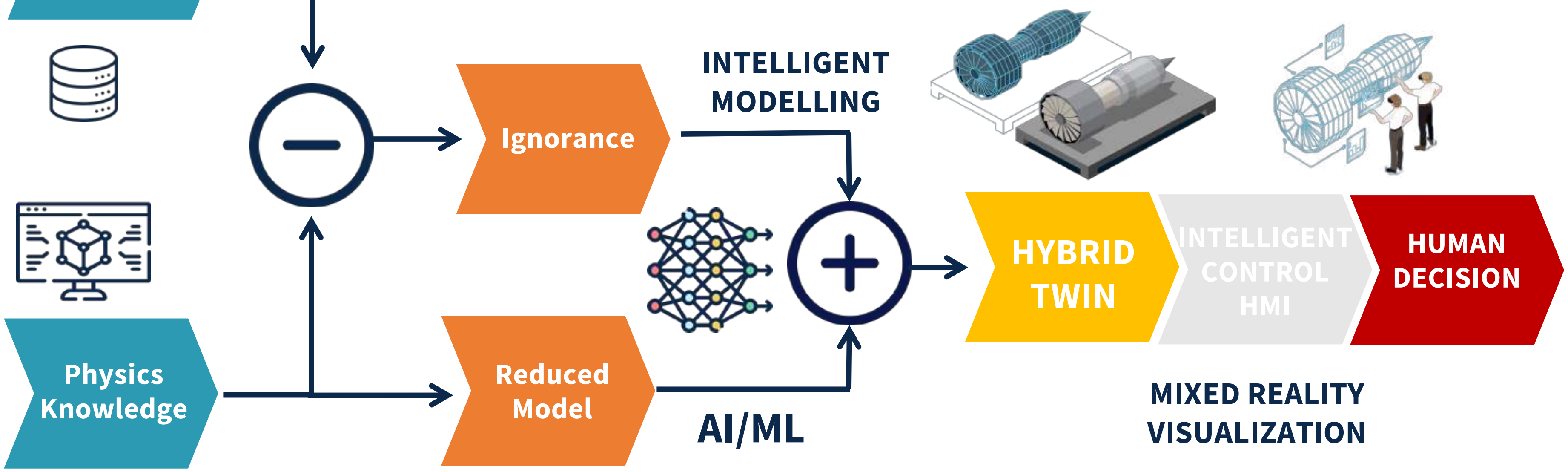
PATENTS FILLED

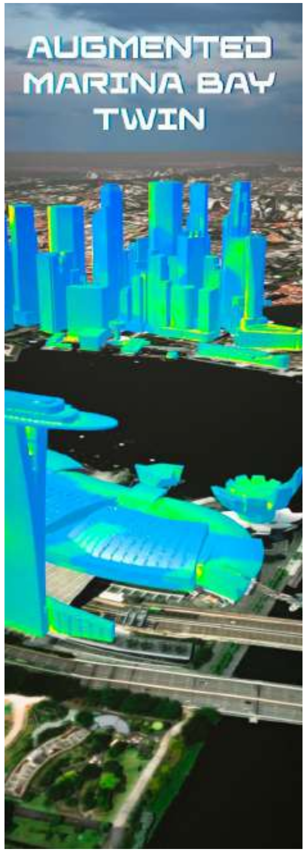
1

START-UP CREATED

HYBRID TWIN APPROACH

$$\frac{dx}{dt} = f^{\texttt{physics-based}}(x, \mathbf{z}) + f^{\texttt{data-driven}}(x, \mathbf{z})$$





CONTEXT
Environmental conditions are strongly impacted by the wind field: temperature, noise, air quality, pollutant dispersion, …

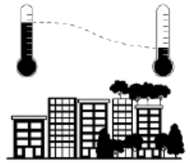
OBJECTIVE
Computing the wind map and all the associated environmental fields

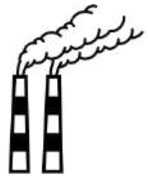
APPROACH
Surrogates working on **parametric** maps

OUTCOME
Parametric environmental real-time models

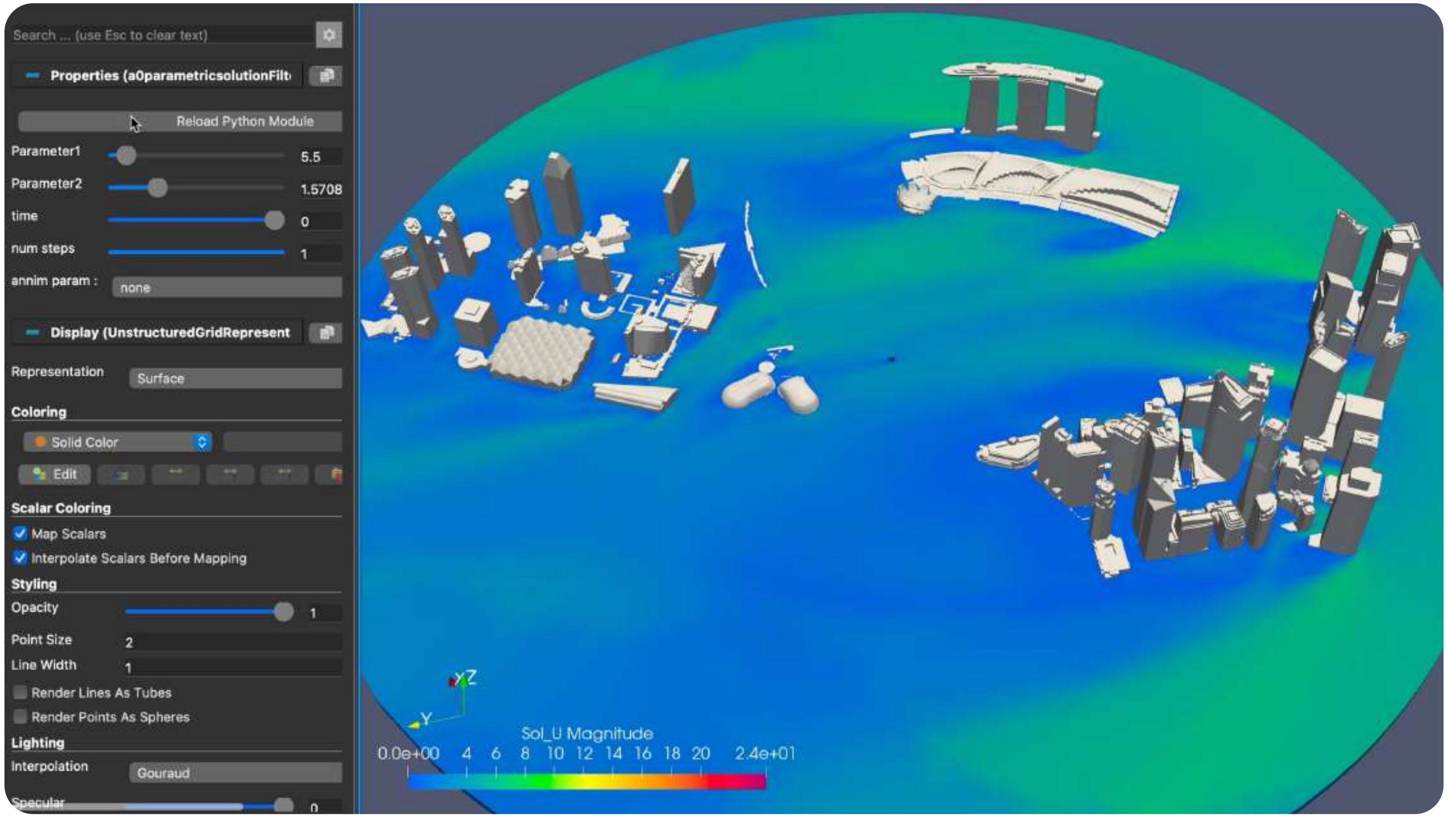
WIND MAP


ISKANDAR PUTERI
E3
E3
PIE
Singapore
QPG
SINGAPORE
CHANGI AIRPORT
Nanyang Technological
University
KPE
KPE
National University
of Singapore





WIND MAP: DOWNSCALING

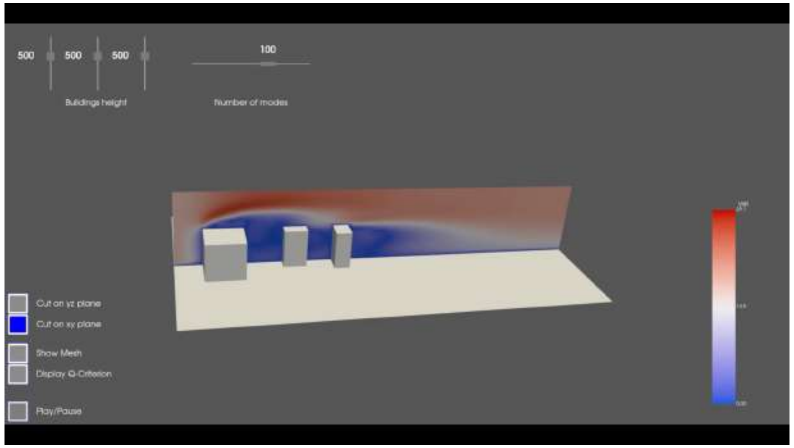


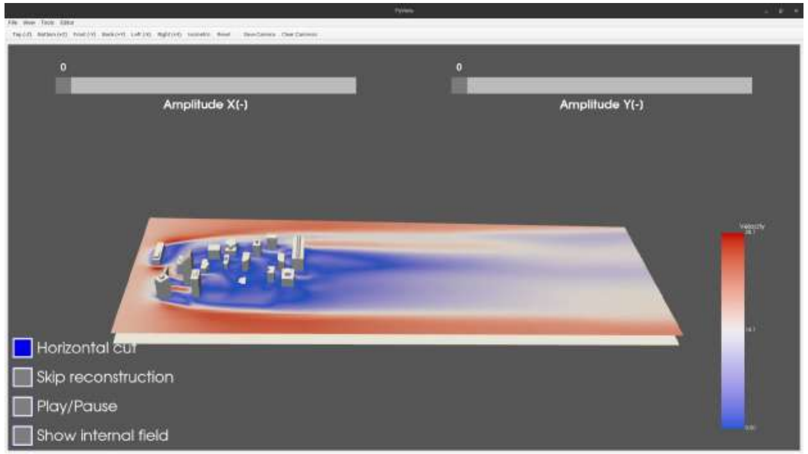
duoverse

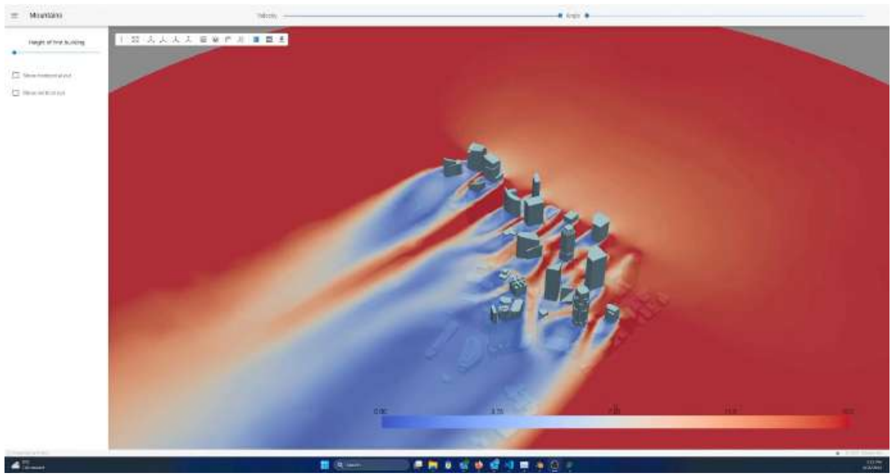
Bridge the gap between models and reality.

OpenFOAM

MAPS FOR PLANNING





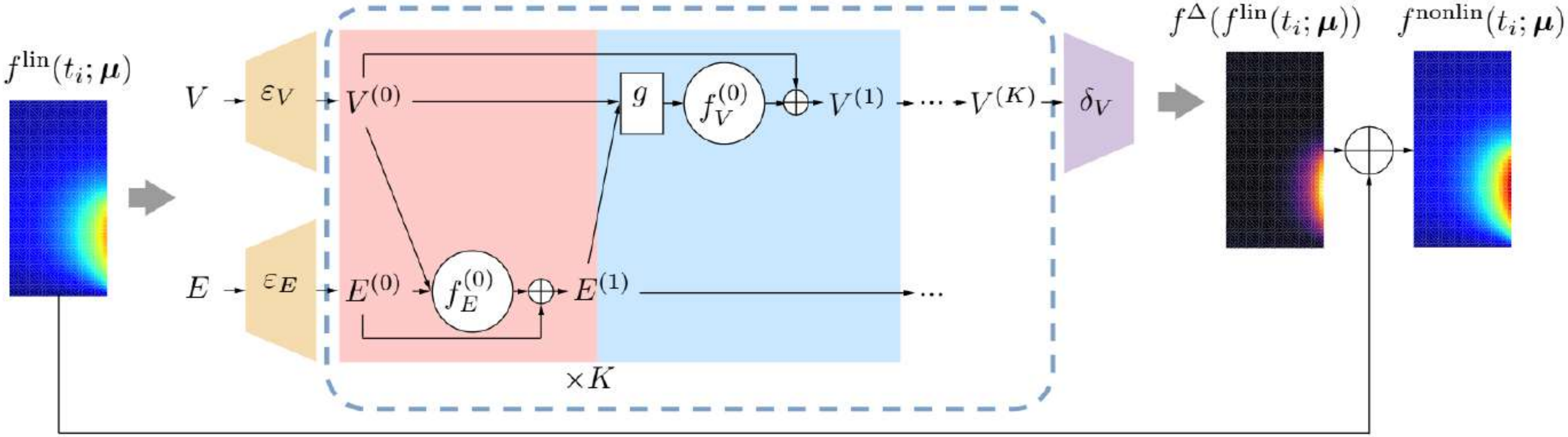


duoverse

Bridge the gap between models and reality.

OpenFOAM

$$f^{\mathrm{GT}}(t;\boldsymbol{\mu}) = f^{\mathrm{FEM}}(t;\boldsymbol{\mu}) + f^{\Delta}(f^{\mathrm{FEM}}(t;\boldsymbol{\mu}))$$



$$\mathbf{h}_{v_i}^{(0)} = \varepsilon_V(\mathbf{v}_i;\boldsymbol{\Theta}_{\varepsilon_V})$$

$$\mathbf{y}_i = \delta_V(\mathbf{h}_{v_i}^{(K)};\boldsymbol{\Theta}_{\delta_V})$$

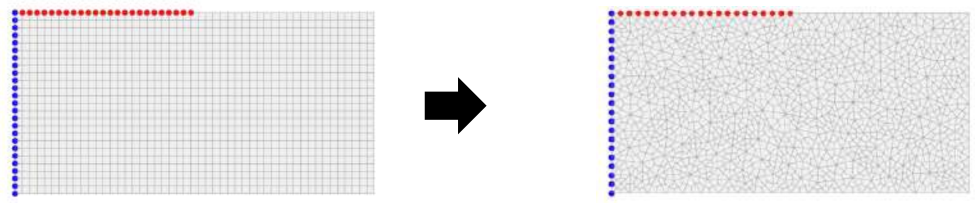
$$\mathbf{h}_{e_{ij}}^{(0)} = \varepsilon_E(\mathbf{e}_{ij};\boldsymbol{\Theta}_{\varepsilon_E})$$

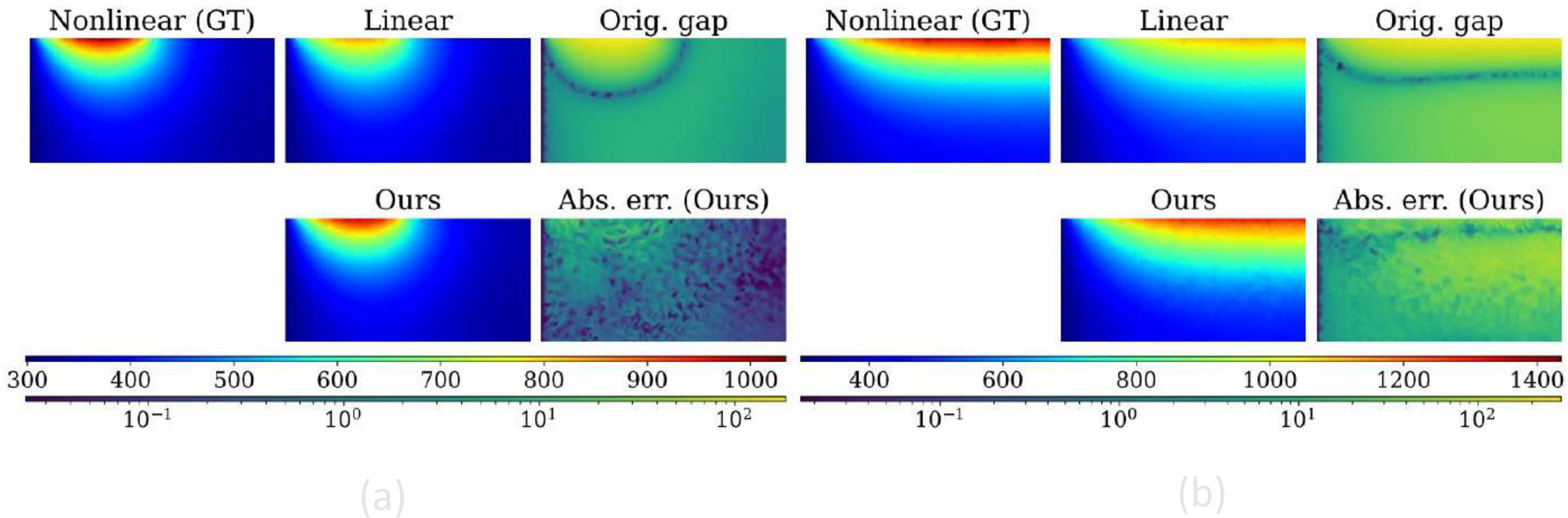
$$\mathbf{h}_{e_{ij}}^{(k+1)} = \mathbf{h}_{e_{ij}}^{(k)} + f_E^{(k)}\left(\mathbf{h}_{e_{ij}}^{(k)}, \mathbf{h}_{v_i}^{(k)}, \mathbf{h}_{v_j}^{(k)}; \boldsymbol{\Theta}_{f_E^{(k)}}\right)$$

$$\mathbf{h}_{v_i}^{(k+1)} = \mathbf{h}_{v_i}^{(k)} + f_V^{(k)}\left(\mathbf{h}_{v_i}^{(k)}, \mathbf{g}\left(\left\{\mathbf{h}_{e_{ij}}^{(k+1)} \mid j \in \mathcal{N}(i)\right\}\right); \boldsymbol{\Theta}_{f_V^{(k)}}\right)$$

Bridging Data and Physics: A Graph Neural Network–Based Hybrid Modeling Framework for FEM approximations. M. Gorpinich, B. Moya, S. Rodriguez, F. Meraghni, Y. Jaafra, A. Briot M. Henner, R. Leon, F. Chinesta

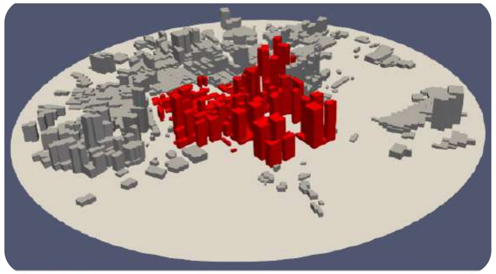
Mesh generalization

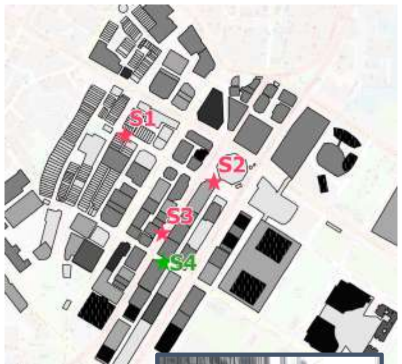


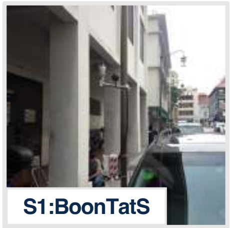


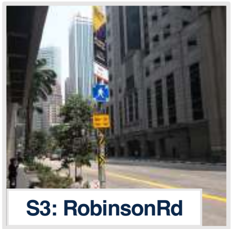
Prediction of the simulation on an irregular mesh with the training performed on the regular mesh.

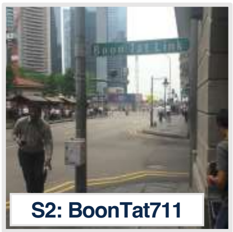
HYBRID MODELLING: IMPROVING PREDICTIONS ACCURACY

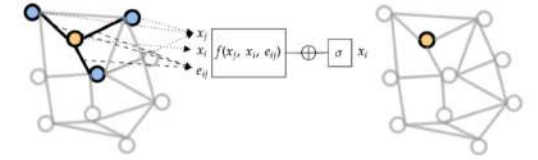












$$x_i^{(l)} = \sigma^{(l)}\left(x_i^{(l-1)}, \bigoplus_{j\in\mathcal{N}(v_i)} f^{(l)}(x_i^{(l-1)}, x_j^{(l-1)}, e_{ij}^{(l-1)})\right),$$

$$x_i^{(l)} = \psi^{(l)}(x_i^{(l-1)}, x_j^{(l-1)}, e_{ij}^{(l-1)})$$

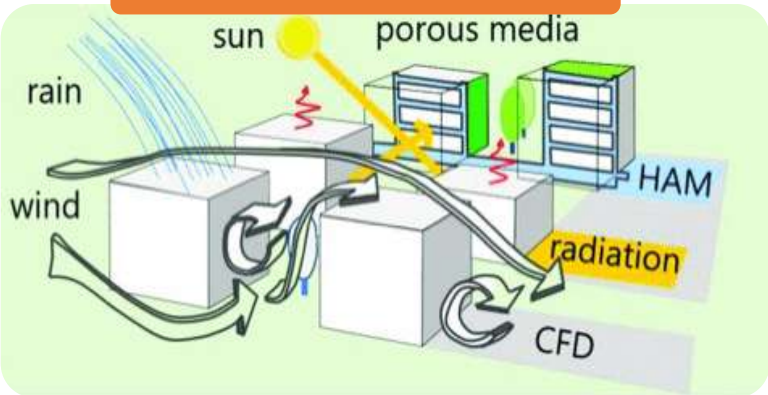
Root Mean Square Error (°C)	Measurement sites			
	S1 (temporal validation)	S2 (temporal validation)	S3 (temporal validation)	S4 (spatial validation)
SURROGATE	1.3	2.1	1.9	1.7
HYBRID	**0.6**	**0.7**	**0.6**	**0.7**

Hybrid Model improves performance & corrects inaccuracies

DesCartes

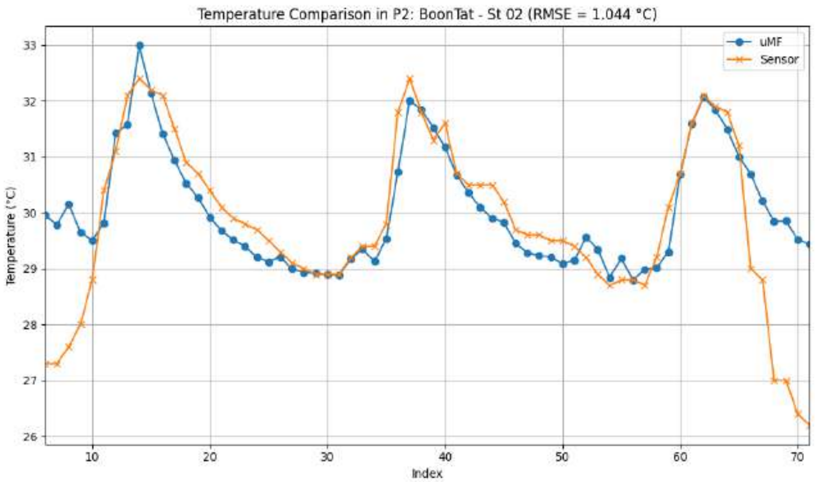
TEMPERATURE: OUTDOOR (AUG. 2025 – AUG. 2026)

SIMULATION MODEL



VS

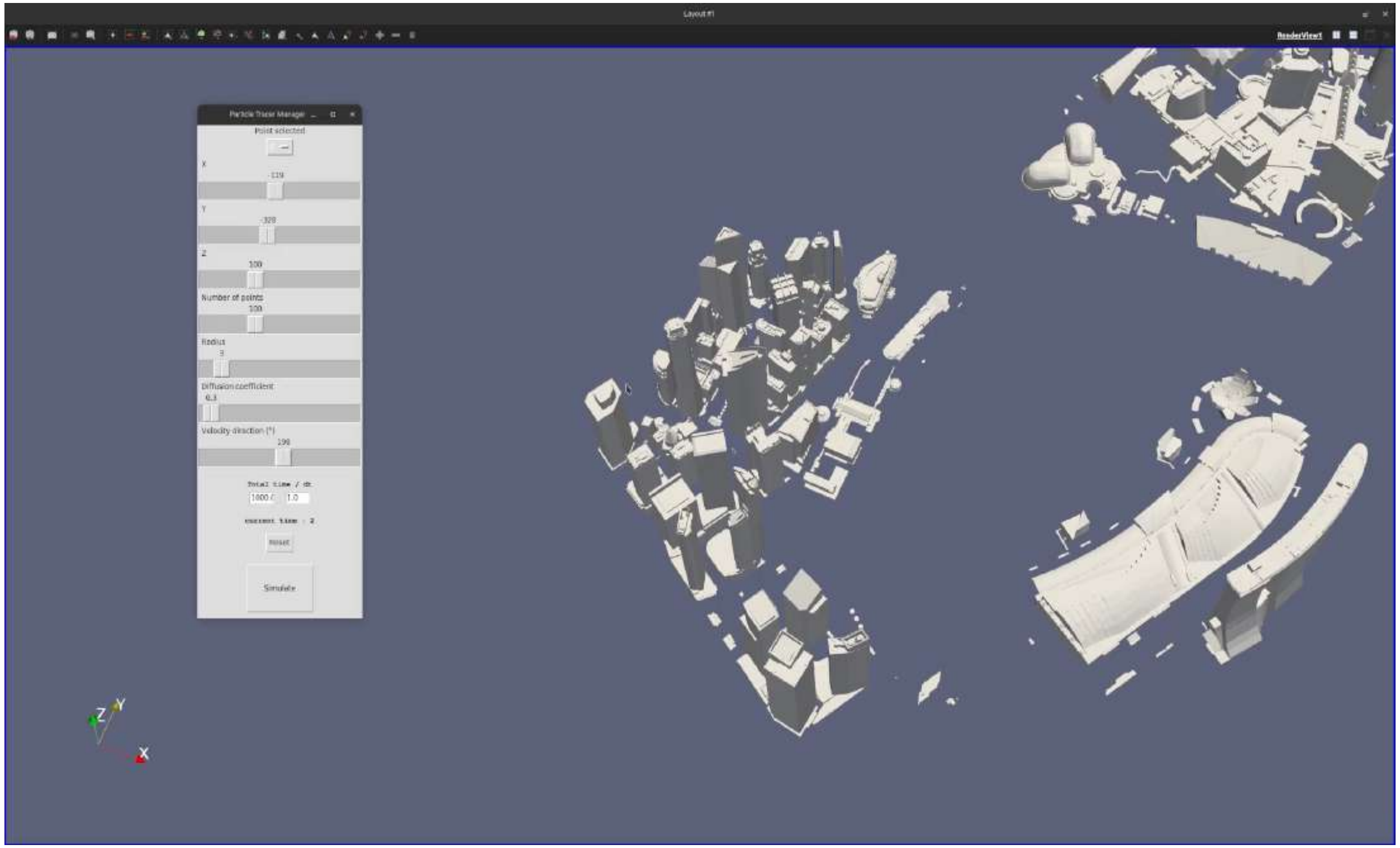
REAL DATA (FROM COOLING SINGAPORE)



SUCCESSFUL PREDICTION!

(SEC) SINGAPORE-ETH CENTRE

RISK EVALUATION: POLLUTION DISPERSION



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Bridge the gap between models and reality.

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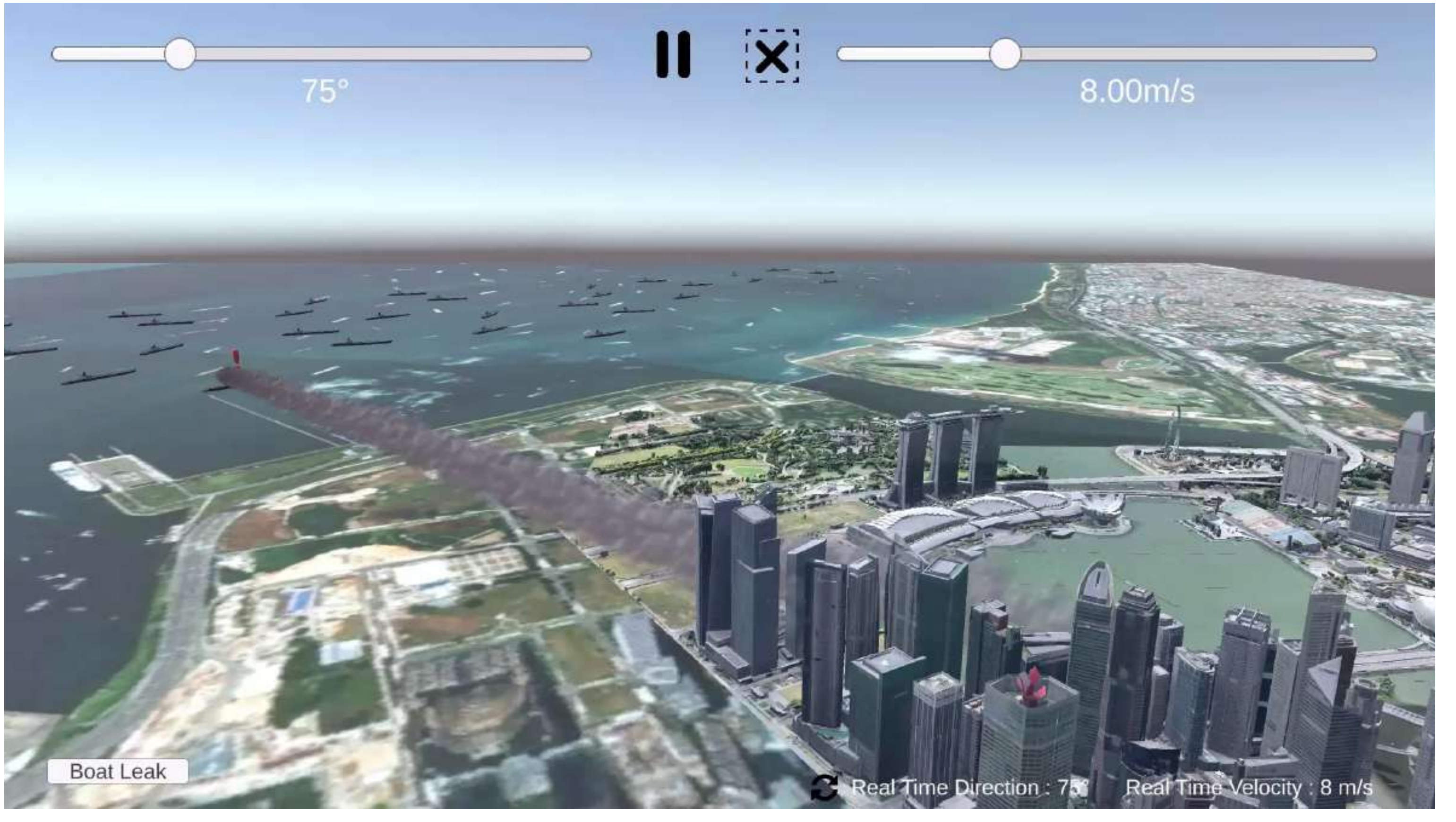
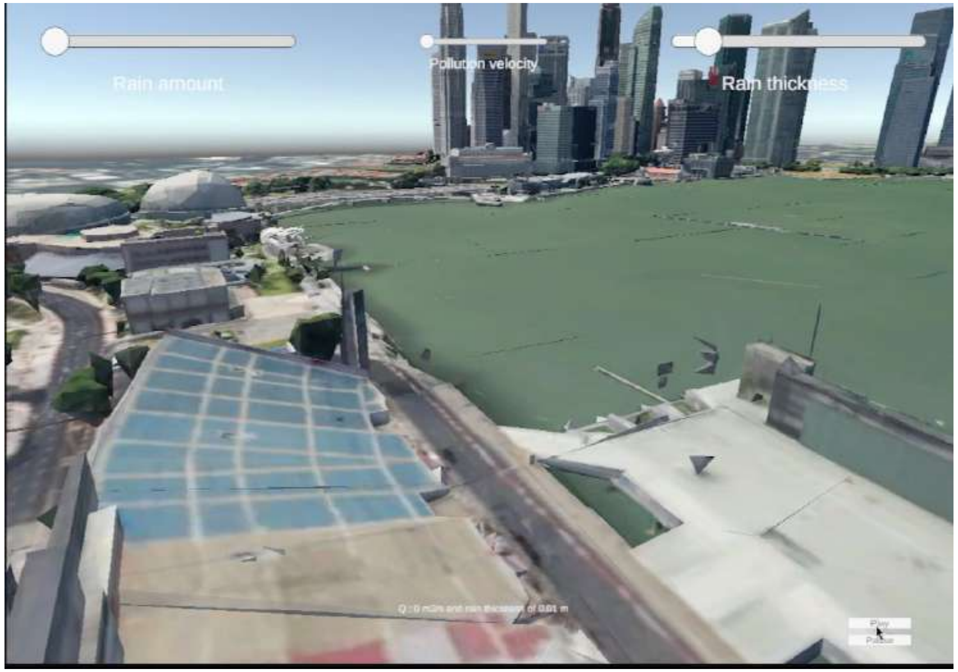
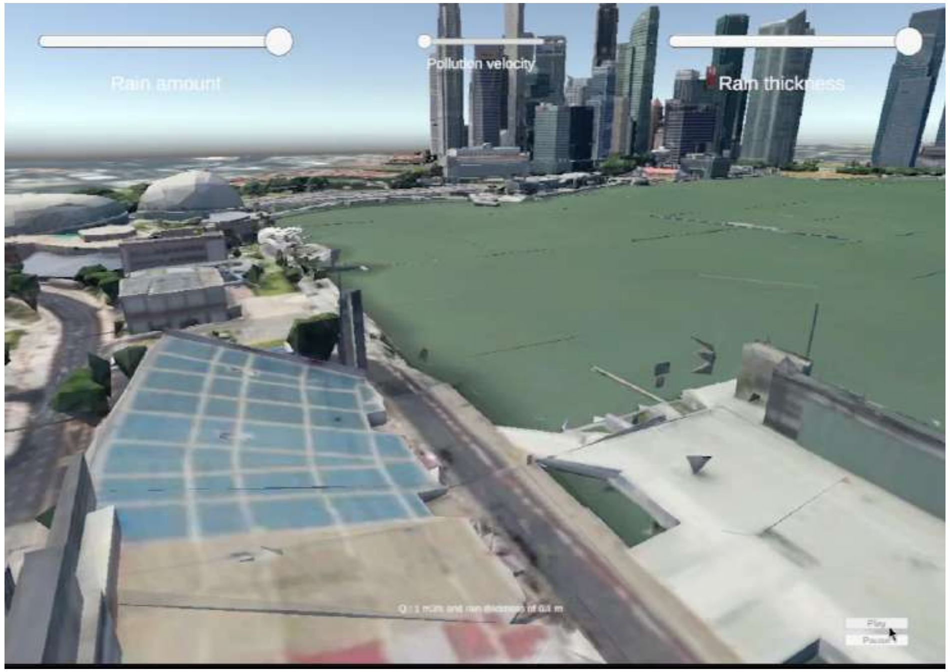
RISK EVALUATION: PLUME DISPERSION



Bridge the gap between models and reality.

RISK MITIGATION





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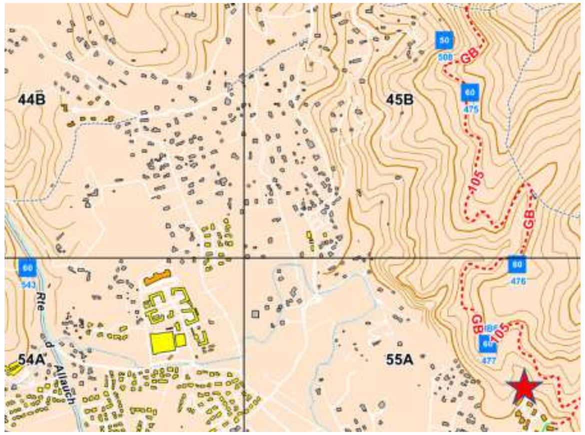
RISK EVALUATION: OIL DISPERSION

RISK MANAGEMENT: FIRE PROPAGATION



MARINS POMPIERS
MARSEILLE

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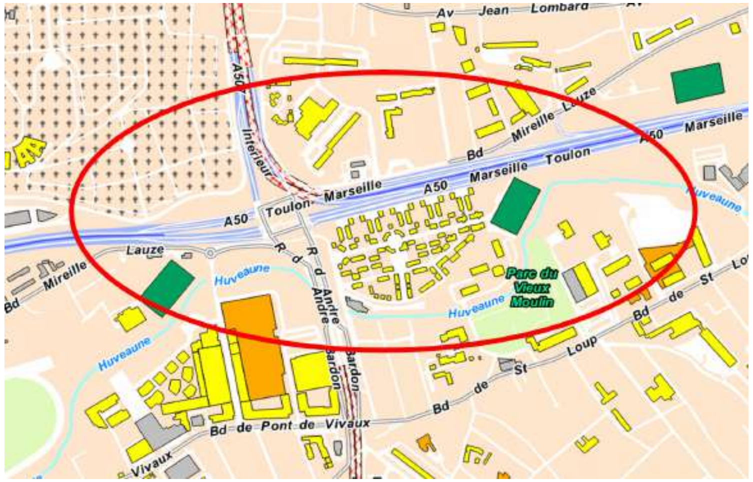
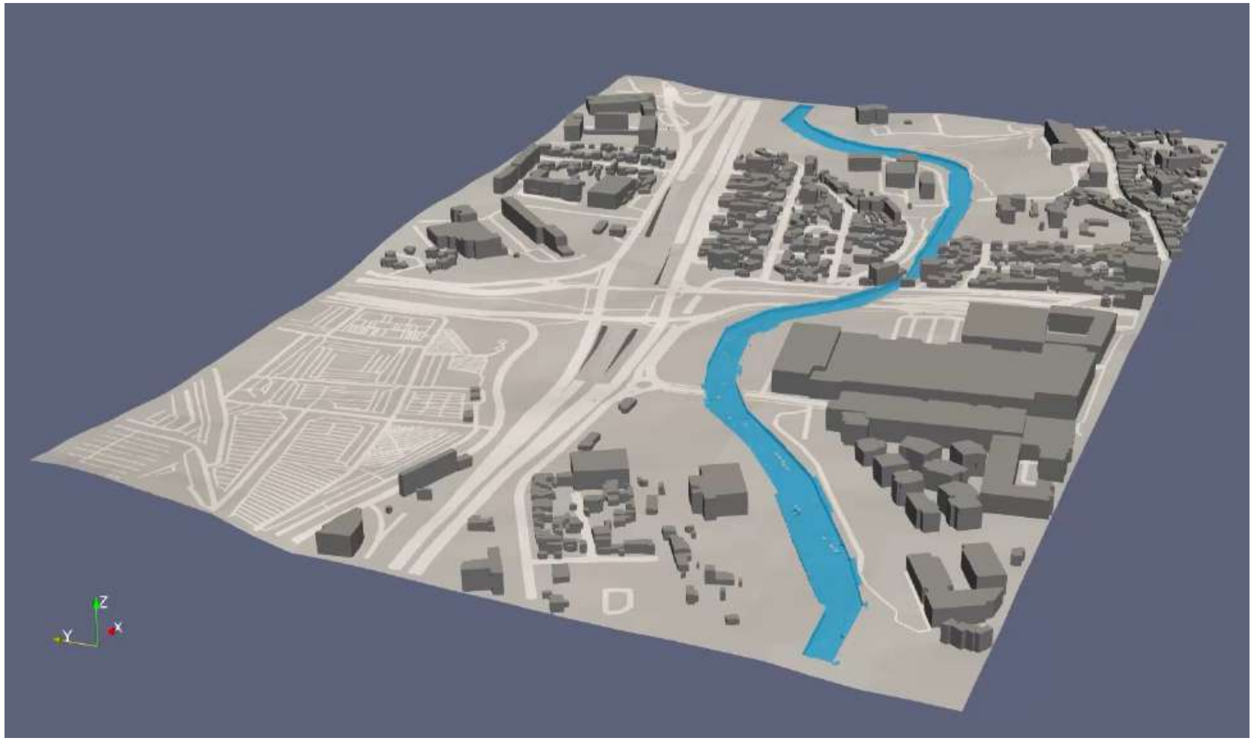
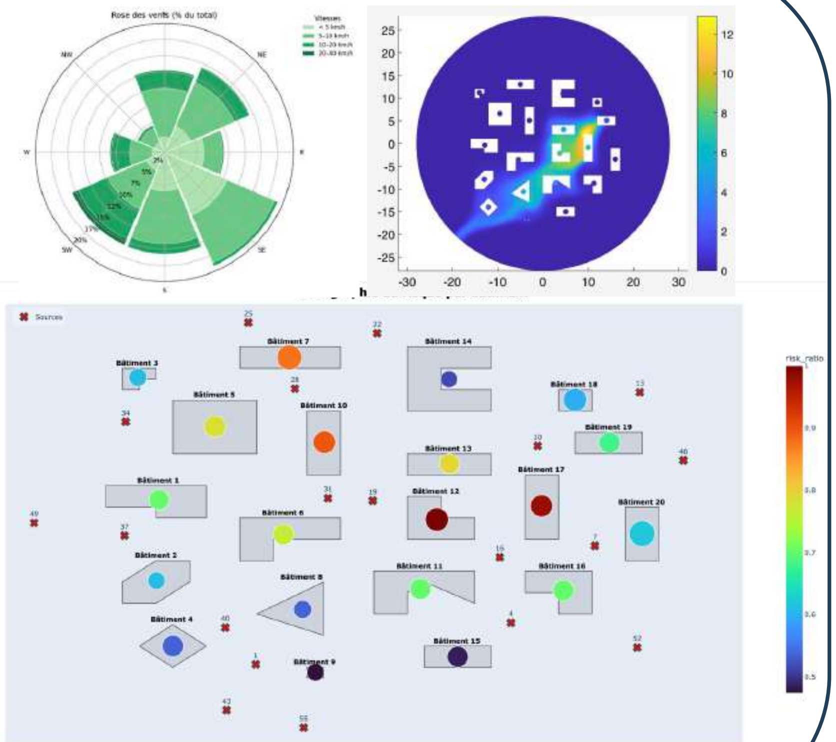
RISK MANAGEMENT: FLOODING





HYBRID MODELS – RISK – ECONOMICAL IMPACT: INSURANCES



Conclusions and future work

Conclusions

A smart territory is not over-digitalized. However, its transition is led by hybrid models supported by specific knowledge.

Next steps- towards enhanced manifolds: Interpretable spaces with coherent results and uncertainty. Construction of KPIs for risk evaluation.

ACKNOWLEDGEMENTS

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ADVANCES IN HYBRID MODELING: TOWARDS THE NUMERICAL TRANSITION OF TERRITORIES

Beatriz Moya, Alicia Tierz, Huangbin Liang, Ruben Laurenco, Jad Mounayer, Sebastian Rodriguez, David Gonzalez, Iciar Alfaro, Elias Cueto, Eleni Chatzi, Francisco Chinesta