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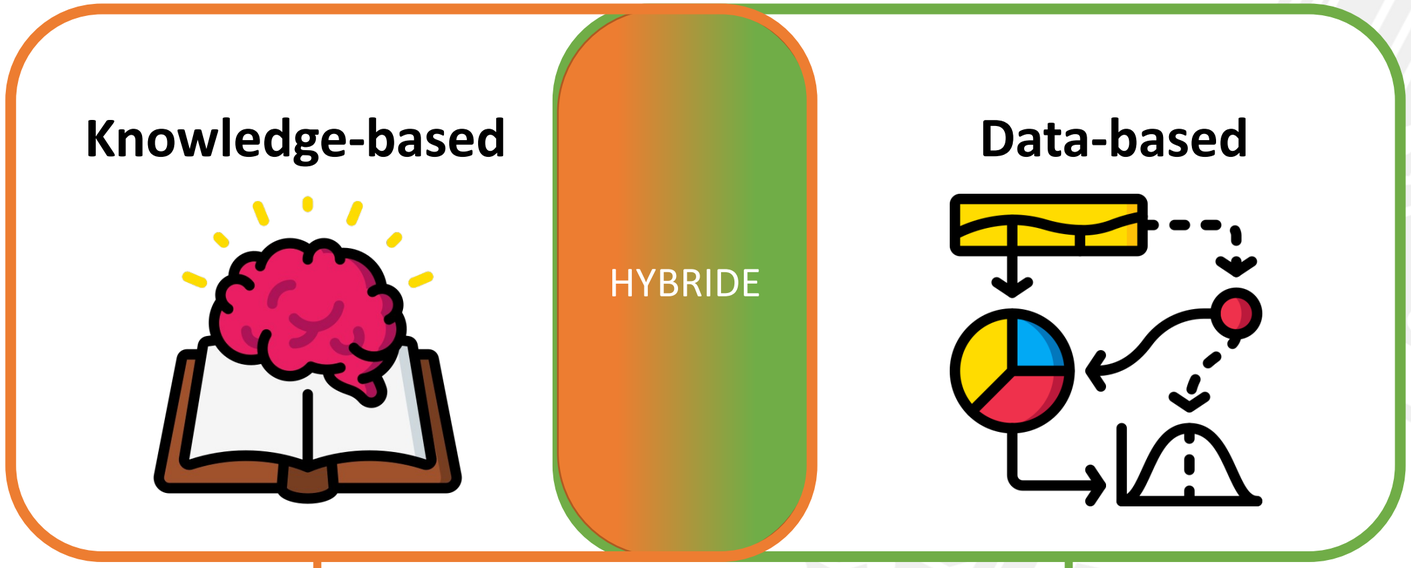
CONNAISSANCE & INTELLIGENCE ARTIFICIELLE DISTRIBUÉES

Sarah Ghidalia - PFIA 2024

Introduction au Physics-Informed Machine Learning

Github

https://github.com/Mileem/PFIA_2024



Connaissance
Systèmes Expert
Ontologies

Données
Machine Learning
Deep Learning

Historique de l'IA Hybride

- R. Sun, "Robust reasoning: integrating rule-based and similarity-based reasoning," Artificial Intelligence, vol. 75, no. 2, pp. 241–295, Jun. 1995, doi: 10.1016/0004-3702(94)00028-Y.

- A. S. d'Avila Garcez, K. B. Broda, and D. M. Gabbay, Neural-Symbolic Learning Systems. in Perspectives in Neural Computing. London: Springer, 2002. doi: 10.1007/978-1-4471-0211-3.

- S. Bader and P. Hitzler, "Dimensions of Neural-symbolic Integration - A Structured Survey." arXiv, Nov. 10, 2005. doi: 10.48550/arXiv.cs/0511042.

Historique de l'IA Hybride

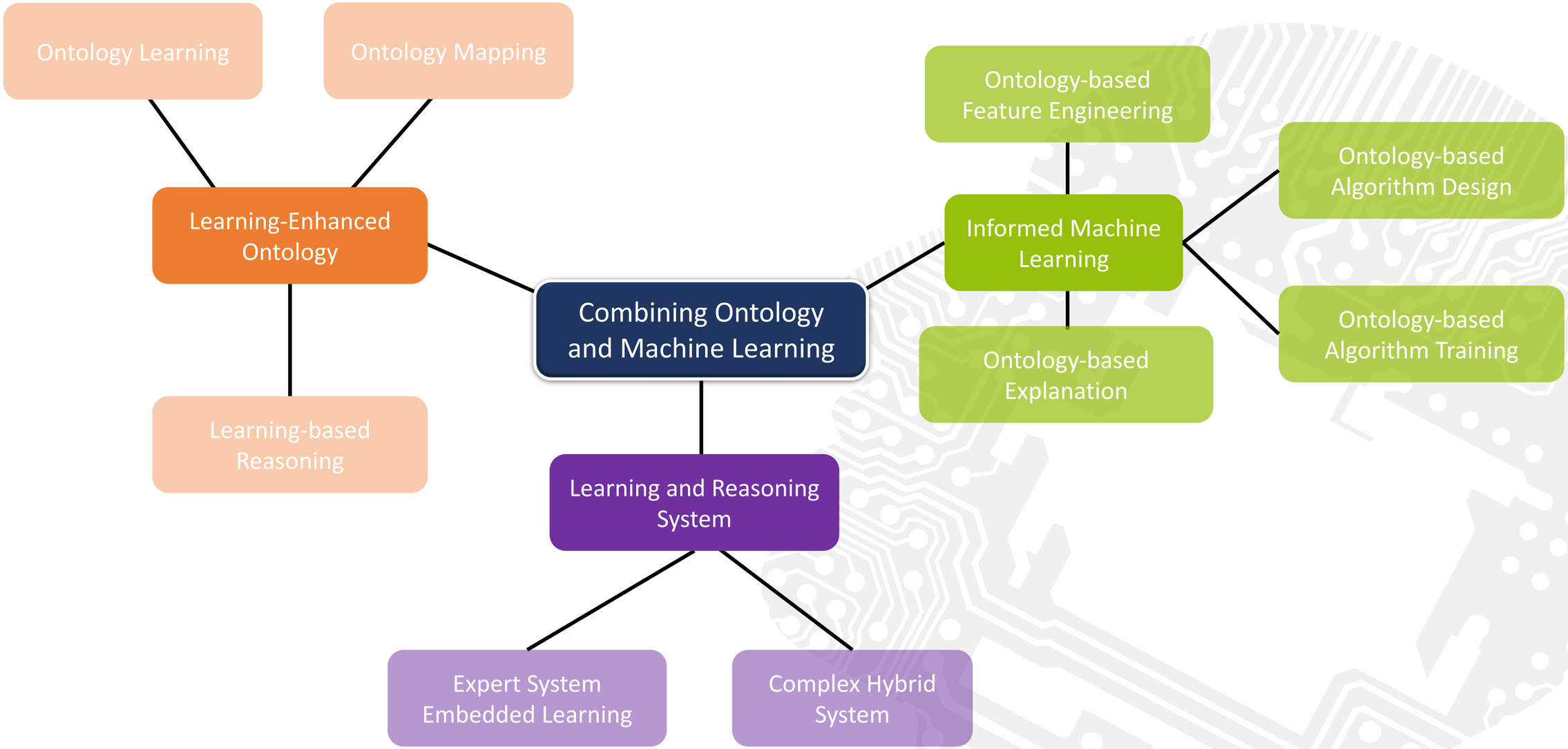
- A. S. d'Avila Garcez and L. C. Lamb, "Neurosymbolic AI: The 3rd Wave." arXiv, Dec. 16, 2020. doi: 10.48550/arXiv.2012.05876.

- G. Marcus, "The Next Decade in AI: Four Steps Towards Robust Artificial Intelligence." arXiv, Feb. 19, 2020. doi: 10.48550/arXiv.2002.06177.

- H. Kautz, "The Third AI Summer: AAAI Robert S. Engelmore Memorial Lecture," *AI Magazine*, vol. 43, no. 1, Art. no. 1, Mar. 2022, doi: 10.1002/aaai.12036.

- M. van Bekkum, M. de Boer, F. van Harmelen, A. Meyer-Vitali, and A. ten Teije, "Modular Design Patterns for Hybrid Learning and Reasoning Systems: a taxonomy, patterns and use cases," arXiv:2102.11965 [cs], Mar. 2021, Available: http://arxiv.org/abs/2102.11965

Modèles combinant apprentissage automatique et ontologies



Sarah Ghidalia, Ouassila Labbani Narsis, Aurélie Bertaux, Christophe Nicolle. **Combining Machine Learning and Ontology: A Systematic Literature Review.** 2024. ⟨hal-04373122v2⟩

Idée générale: *Theory-guided Data Science*

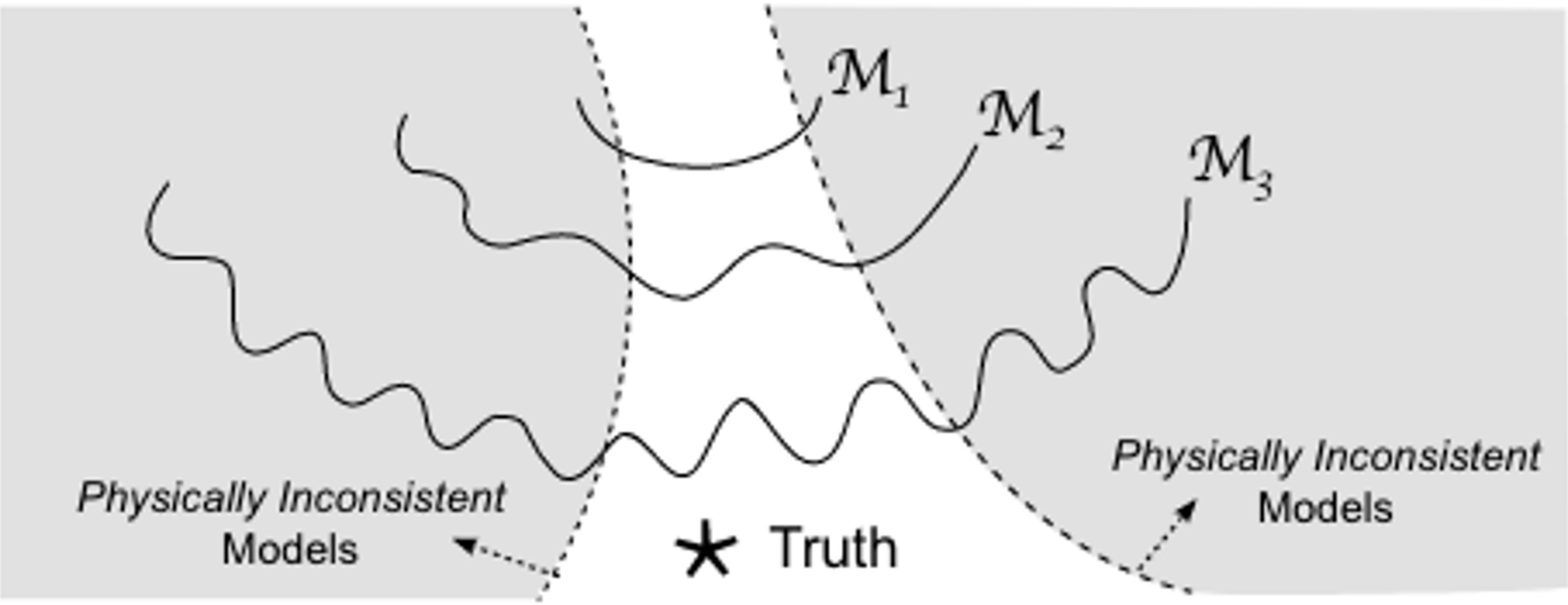


Fig. 2: Scientific knowledge can help in reducing the model variance by removing physically inconsistent solutions, without likely affecting their bias.

Source: A. Karpatne *et al.*, "Theory-guided Data Science: A New Paradigm for Scientific Discovery from Data," *IEEE Trans. Knowl. Data Eng.*, vol. 29, no. 10, pp. 2318–2331, Oct. 2017, doi: 10.1109/TKDE.2017.2720168.

Précision n'est pas cohérence !

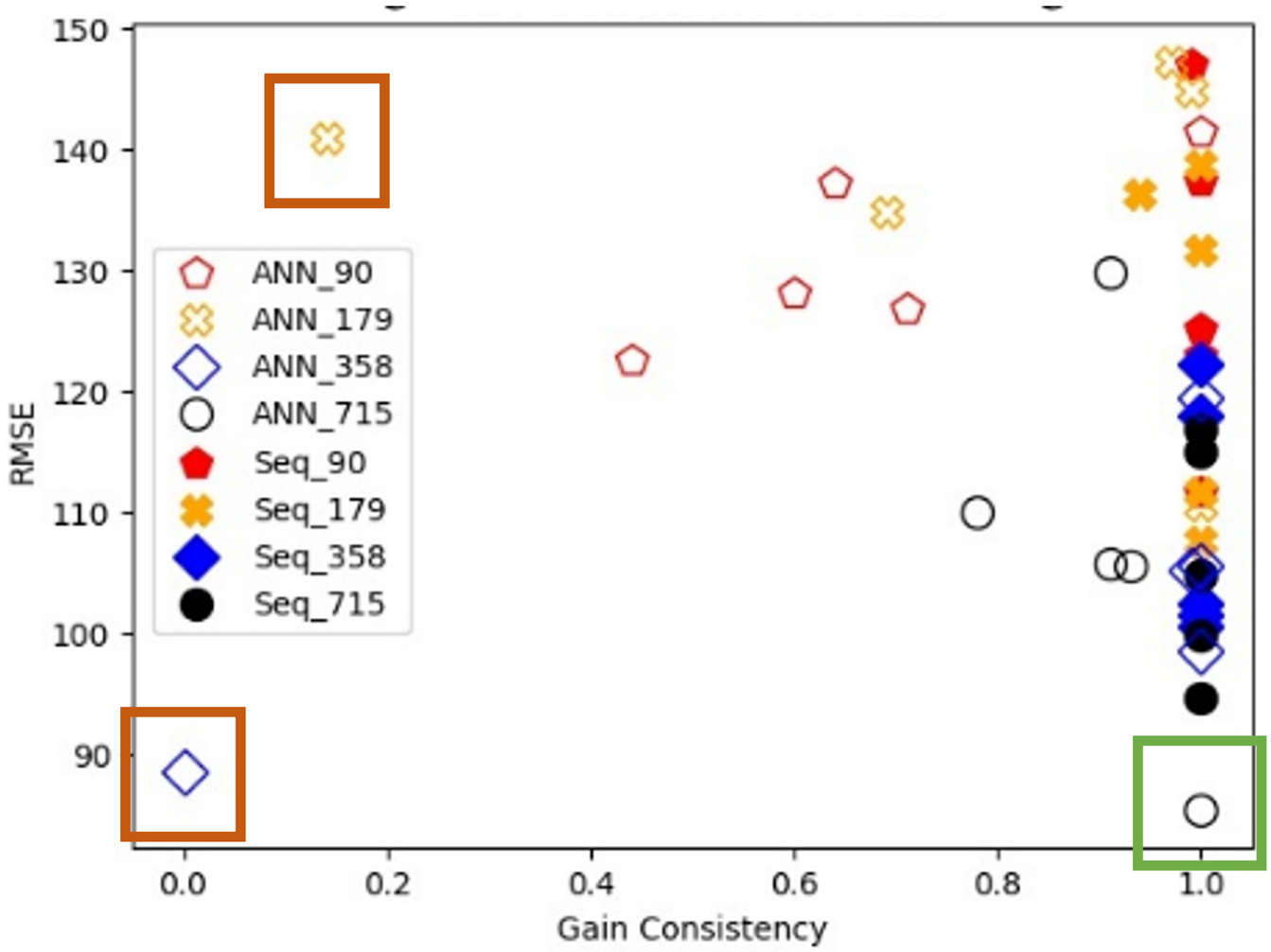
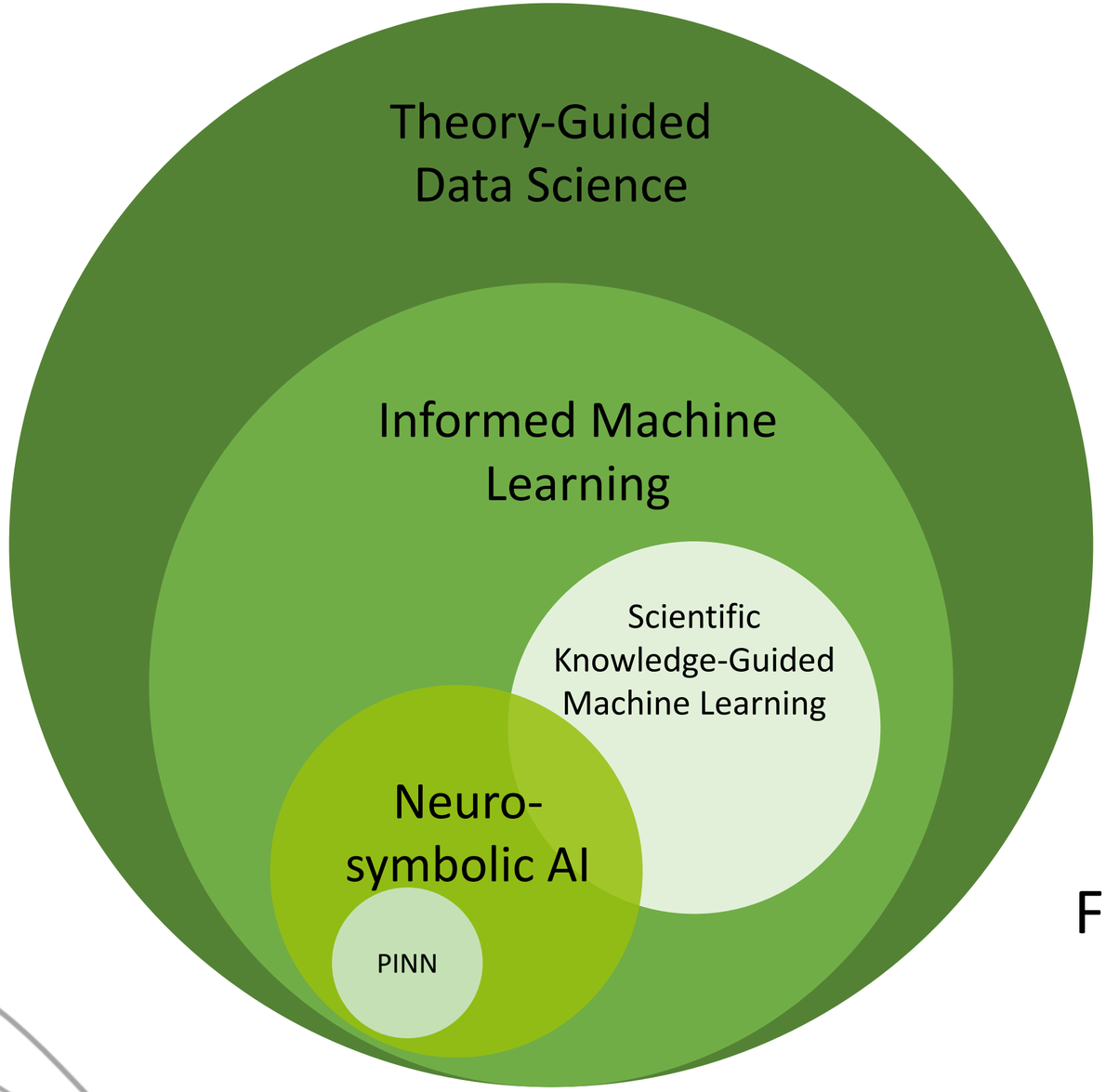


Fig. 9. Process gain consistency vs prediction error of various models for distillate impurity.

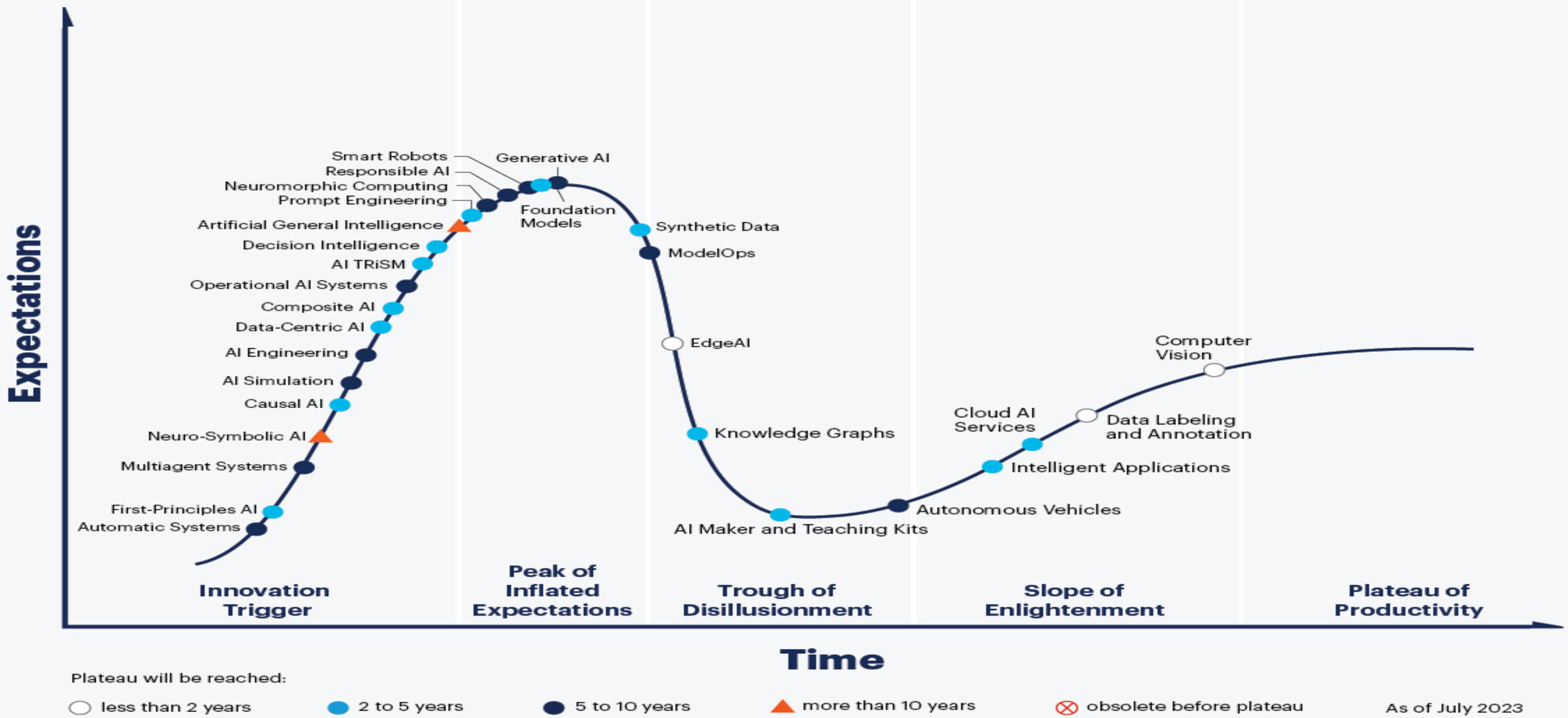
Source: Chou CH, Wu H, Kang JL, et al. *Physically Consistent Soft-Sensor Development Using Sequence-to-Sequence Neural Networks*. IEEE Transactions on Industrial Informatics. 2020;16(4):2829-2838. doi:10.1109/TII.2019.2952429

Vocabulaire



First Principles AI …

Hype Cycle for Artificial Intelligence, 2023



Plateau will be reached:

○ less than 2 years ● 2 to 5 years ● 5 to 10 years ▲ more than 10 years ⊗ obsolete before plateau

As of July 2023

gartner.com

Source: Gartner

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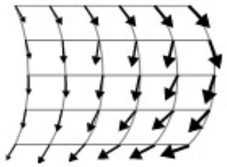
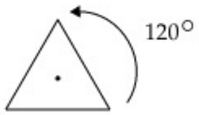
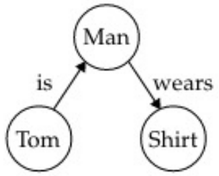
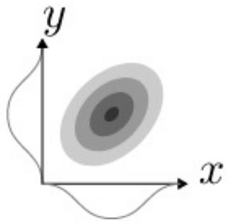
Gartner

Les différentes formes de connaissance …

Table 1: **Illustrative Overview of Knowledge Representations in the Informed Machine Learning Taxonomy.** Each representation type is illustrated by a simple or prominent example in order to give a first intuitive understanding.

Algebraic Equations	Differential Equations	Simulation Results	Spatial Invariances	Logic Rules	Knowledge Graphs	Probabilistic Relations	Human Feedback
$E = m \cdot c^2$ $v \leqslant c$	$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$ $F(x) = m \frac{d^2 x}{dt^2}$			$A \wedge B \Rightarrow C$			

Source: L. von Rueden *et al.*, “Informed Machine Learning -- A Taxonomy and Survey of Integrating Knowledge into Learning Systems,” *IEEE Trans. Knowl. Data Eng.*, pp. 1–1, 2021, doi: 10.1109/TKDE.2021.3079836.

Où ajouter des connaissances dans l'apprentissage ?

Informed Machine Learning

- Knowledge embedding

DONNÉES D'ENTRAINEMENT

PHASE D'APPRENTISSAGE

RÉSULTAT FINAL

- Explication des boites noires
- Évaluation de la cohérence

ARCHITECTURE DU MODÈLE

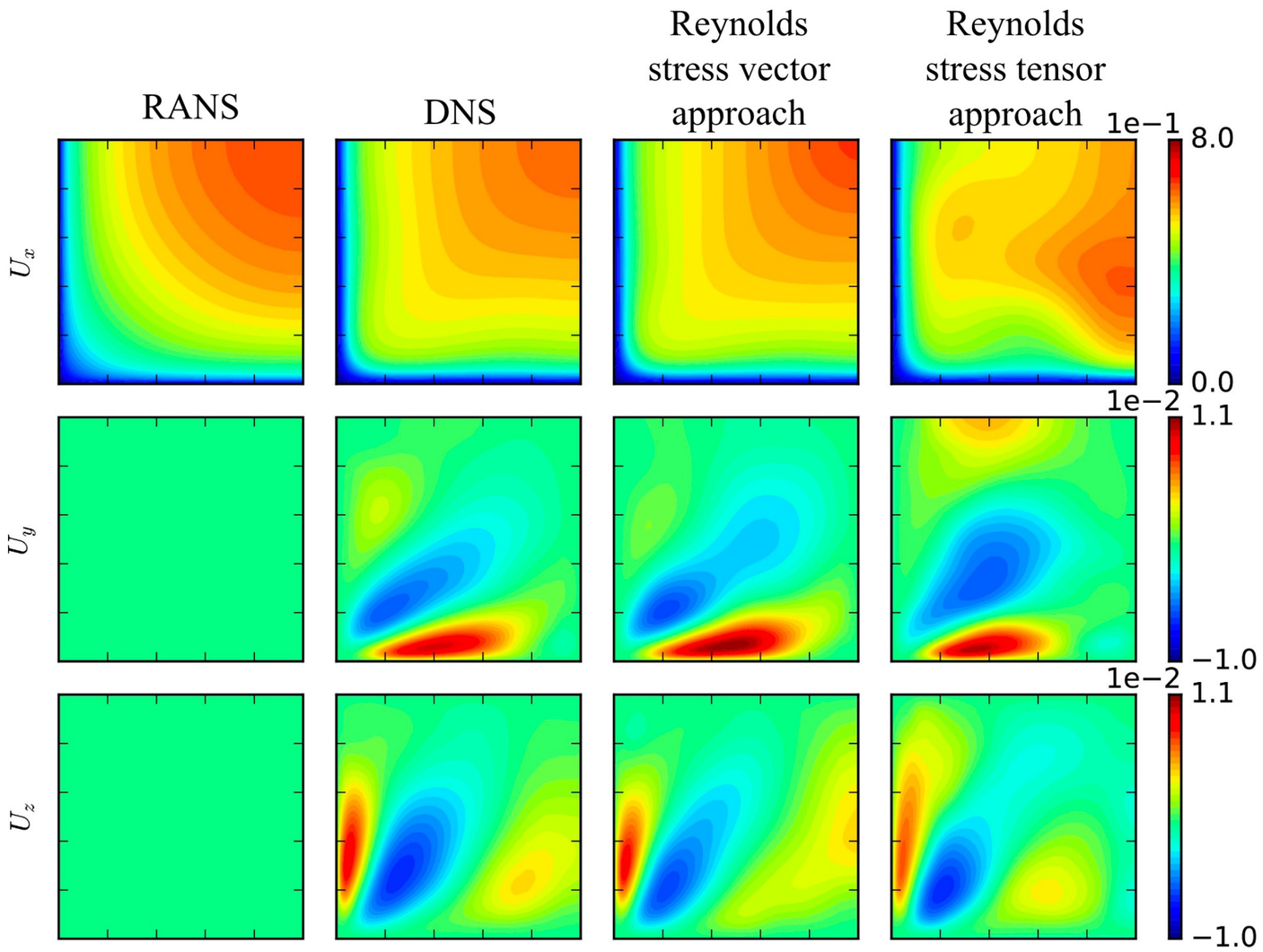
- Fonction de perte

- Graph Neural Network
- Logical Neural Network

Dynamique des fluides

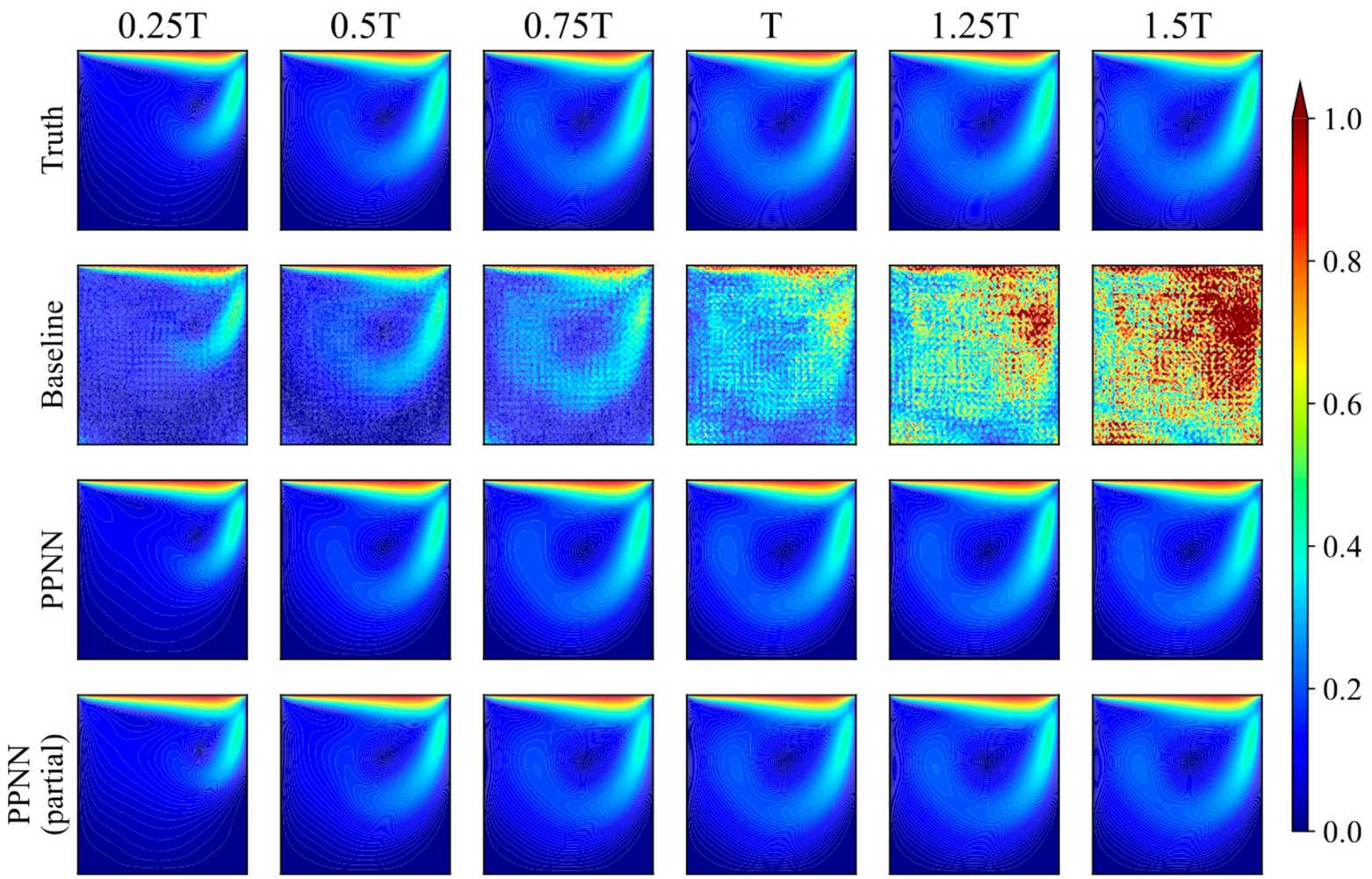
- Modélisation des **turbulences** en aviation (Reynolds-averaged Navier–Stokes)
- Champs d'**éolienne**
- Fabrication de métaux: prédiction de la température et de la dynamique du **bain de fusion**
- Modélisation des **flux cardiovasculaires**
- Débit des **cours d'eau**

Modélisation des Turbulences: Physics-Informed Data



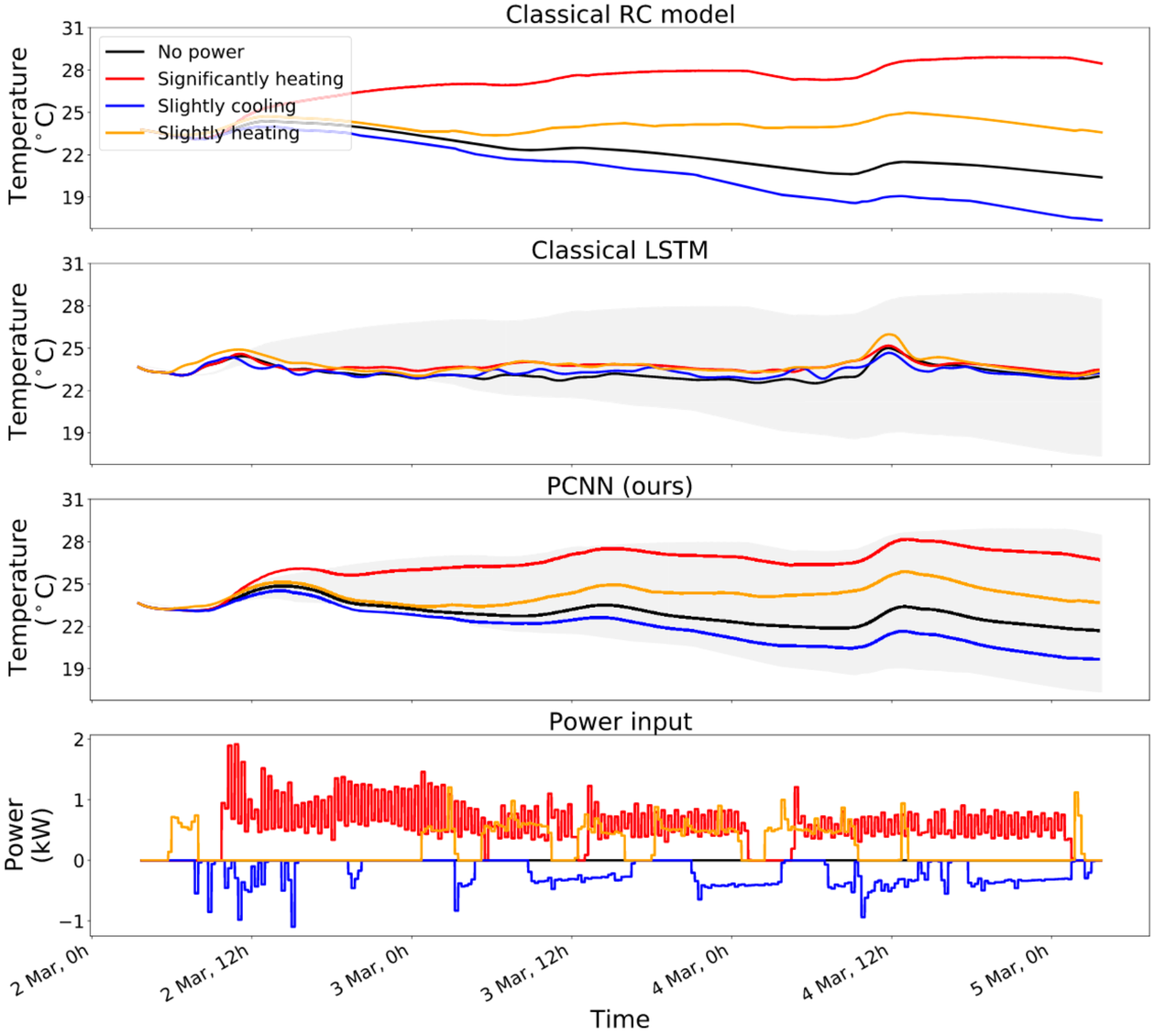
Source: P. Sharma, W. T. Chung, B. Akoush, and M. Ihme, “A Review of Physics-Informed Machine Learning in Fluid Mechanics,” *Energies*, vol. 16, no. 5, Art. no. 5, Jan. 2023, doi: 10.3390/en16052343.

PDE-preserving neural network (PPNN): Physics-Informed Architecture



Source: P. Sharma, W. T. Chung, B. Akoush, and M. Ihme, “A Review of Physics-Informed Machine Learning in Fluid Mechanics,” *Energies*, vol. 16, no. 5, Art. no. 5, Jan. 2023, doi: 10.3390/en16052343.

Batiment: Physics-Informed Learning/Loss



Source: L. Di Natale, B. Svetozarevic, P. Heer, and C. N. Jones, “Physically Consistent Neural Networks for building thermal modeling: Theory and analysis,” *Applied Energy*, vol. 325, p. 119806, Nov. 2022, doi: 10.1016/j.apenergy.2022.119806.

Benchmark: Physics-Informed Evaluation

Table 3: Benchmark result table for the two use cases under 4 categories of evaluation criteria. The performances are reported using three colors computed on the basis of two thresholds. Colors and symbol meaning: 🔴 Not acceptable 🟡 Acceptable 🟢 Great ◎ two problem scales reported (in that case, speed-up for smaller scale is in parenthesis). The number of circles corresponds to the number of variables or laws that are evaluated. For quantitative values from which this table is derived, please refer to section G.1 of appendix and for a color blind version, please refer to Table 11 of appendix.

				Criteria category				
				ML-related		**Readiness**	**OOD Gen.**	**Physics**
			Methods	Quality	Speed-up	Speed-up	Quality	Domain laws
Use cases	Power Grid	Bench1	DC	a 🔴◎	NA	19 (7)	a 🔴◎	P1 🟢◎
			FC	🟢◎	19 (22)	17 (20)	🟡◎	🟡◎
			LeapNet	🟢◎	17 (19)	14 (17)	🟡◎	🟢◎
		Bench2	DC	a p v 🔴🔴🔴	NA	5 (3)	a p v 🔴🔴🔴	P1 P2 P3 P4 P5 P6 P7 P8 🟢🟢🟢🟢🟢🔴🟢🔴
			FC	🟢🟡🟡	99 (157)	57 (27)	🔴🔴🔴	🟡🟡🔴🟢🟡🟢🟢🔴
			LeapNet	🟢🟡🔴	90 (140)	54 (24)	🔴🔴🔴	🟢🟢🔴🟢🟡🔴🟢🔴
	Pneumatic	Bench1	FC	u_Ω 🟢	18	NA	NA	P1 P2 P3 🟡🟡🔴
			UNet	🔴	18	NA	NA	🔴🔴🔴
		Bench2	FC	u_Ω λ_c 🔴🟢	11	NA	u_Ω λ_c 🔴🟢	P1 P2 P3 🔴🟢🟢

M. Leyli Abadi *et al.*, “LIPS - Learning Industrial Physical Simulation benchmark suite,” *Advances in Neural Information Processing Systems*, vol. 35, pp. 28095–28109, Dec. 2022.

Objectifs principaux de l'Informed Machine Learning

- Améliorer la généralisation des modèles d'apprentissage
- Apprendre avec moins de données -> data scarcity
- Garantir la cohérence avec la connaissance
- Meilleure explicabilité

La fonction de perte

$$\mathcal{L} = \mathcal{L}_{data} = | \hat{y} - y |$$

Distance entre les valeurs prédites et les valeurs **observées**

La fonction de perte augmentée par les connaissances

$$\mathcal{L} = \mathcal{L}_{data} + \mathcal{L}_{knowledge}$$

$$\mathcal{L}_{knowledge} = \sum_{i} \lambda_i \mathcal{L}_{knowledge_i}$$

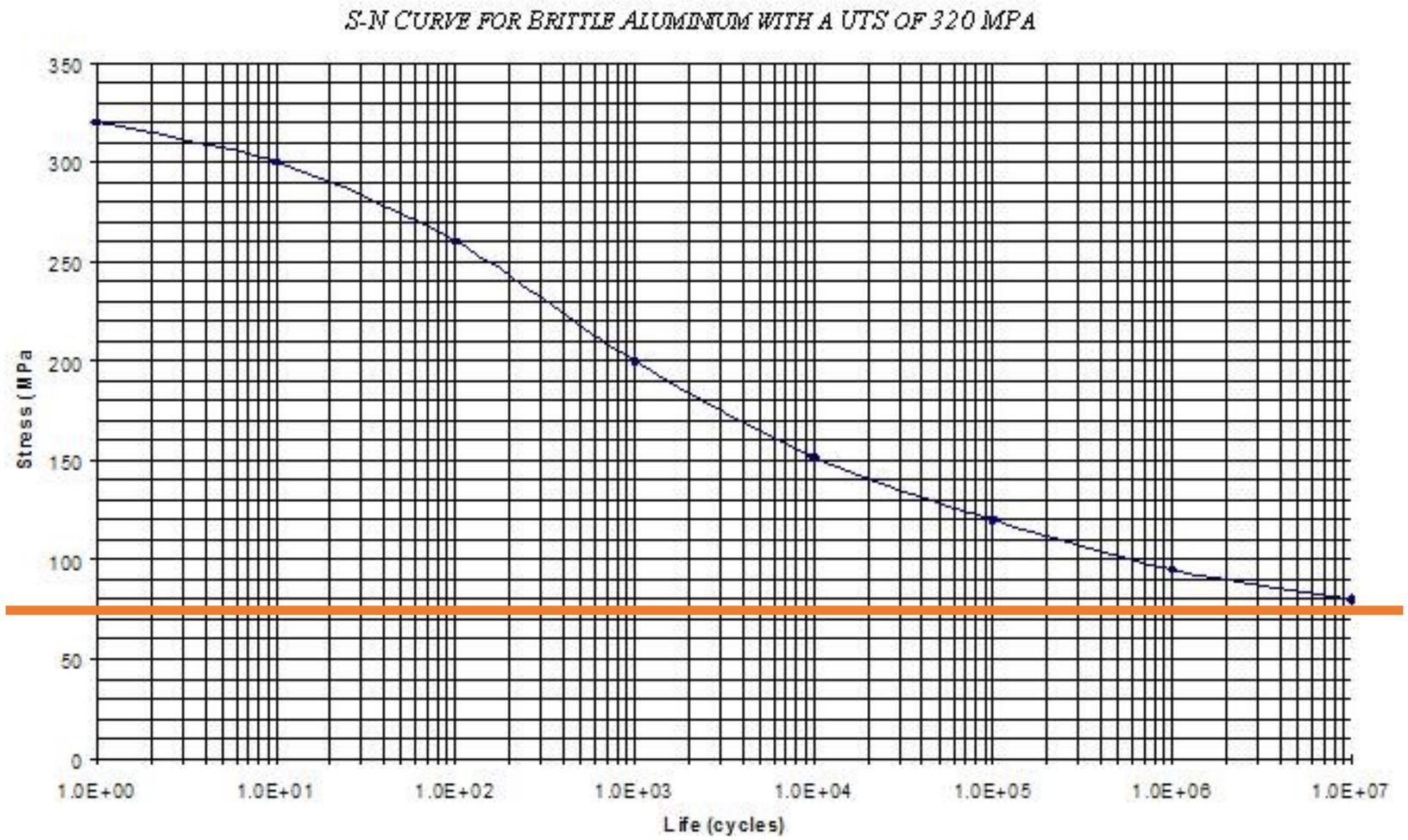
Minimiser un score d'incohérence

Transforme les connaissances en **contraintes**

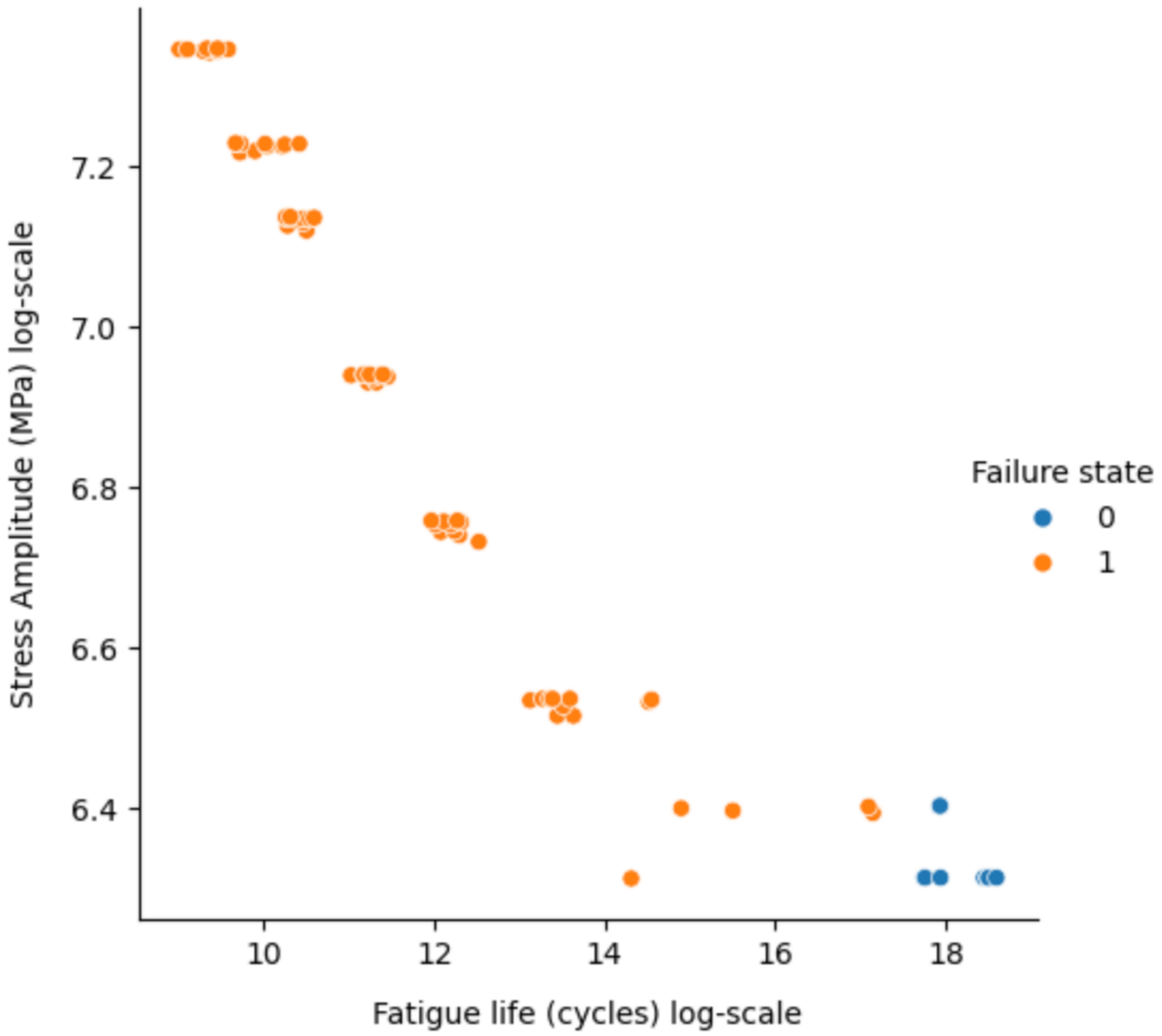
CAS D’USAGE

Un problème de fatigue …

La fatigue des matériaux

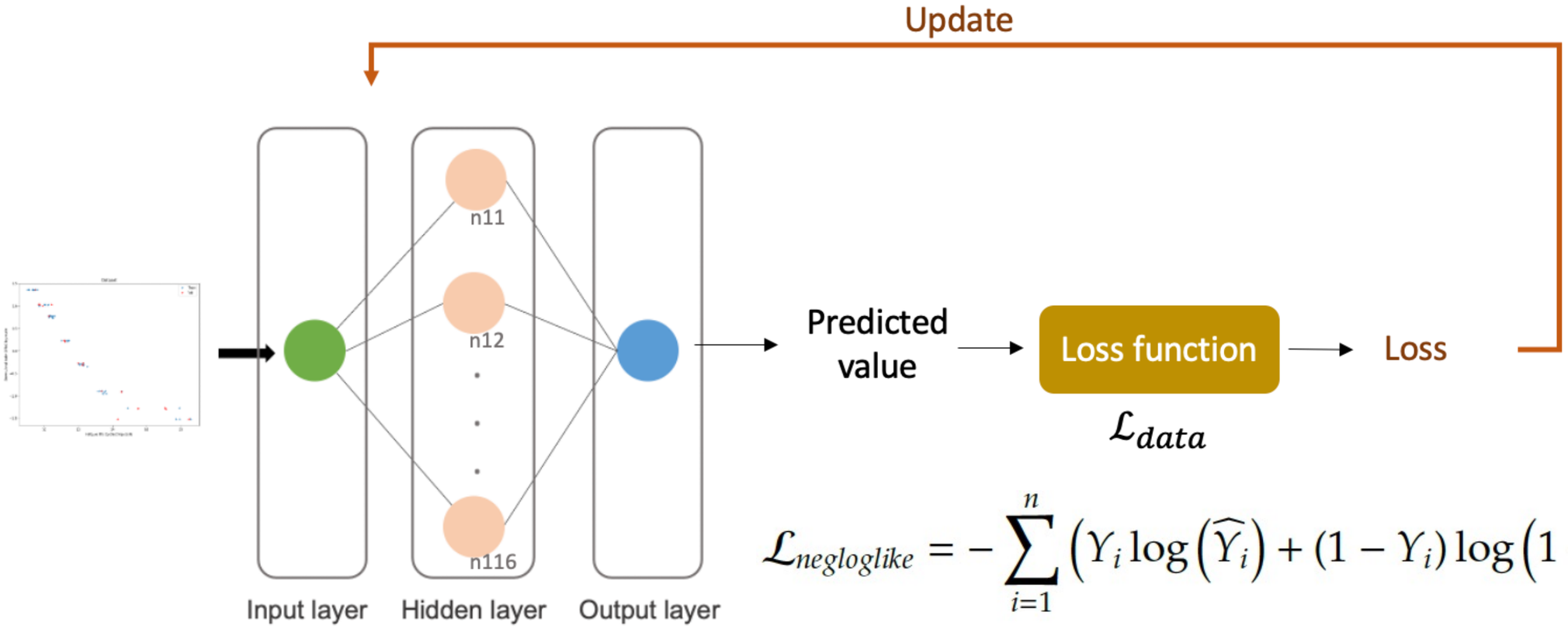


Le cas de l'acier



Étude de la relation entre un **stress** appliqué et la **rupture** d'un matériau pour évaluer sa **résistance**

Neural Network



$\mathcal{L}_{data}$

$$\mathcal{L}_{negloglike} = -\sum_{i=1}^{n}\left(Y_i \log\left(\widehat{Y}_i\right) + (1 - Y_i)\log\left(1 - \widehat{Y}_i\right)\right)$$

Connaissances sur la fatigue des matériaux: Courbe de Wöhler

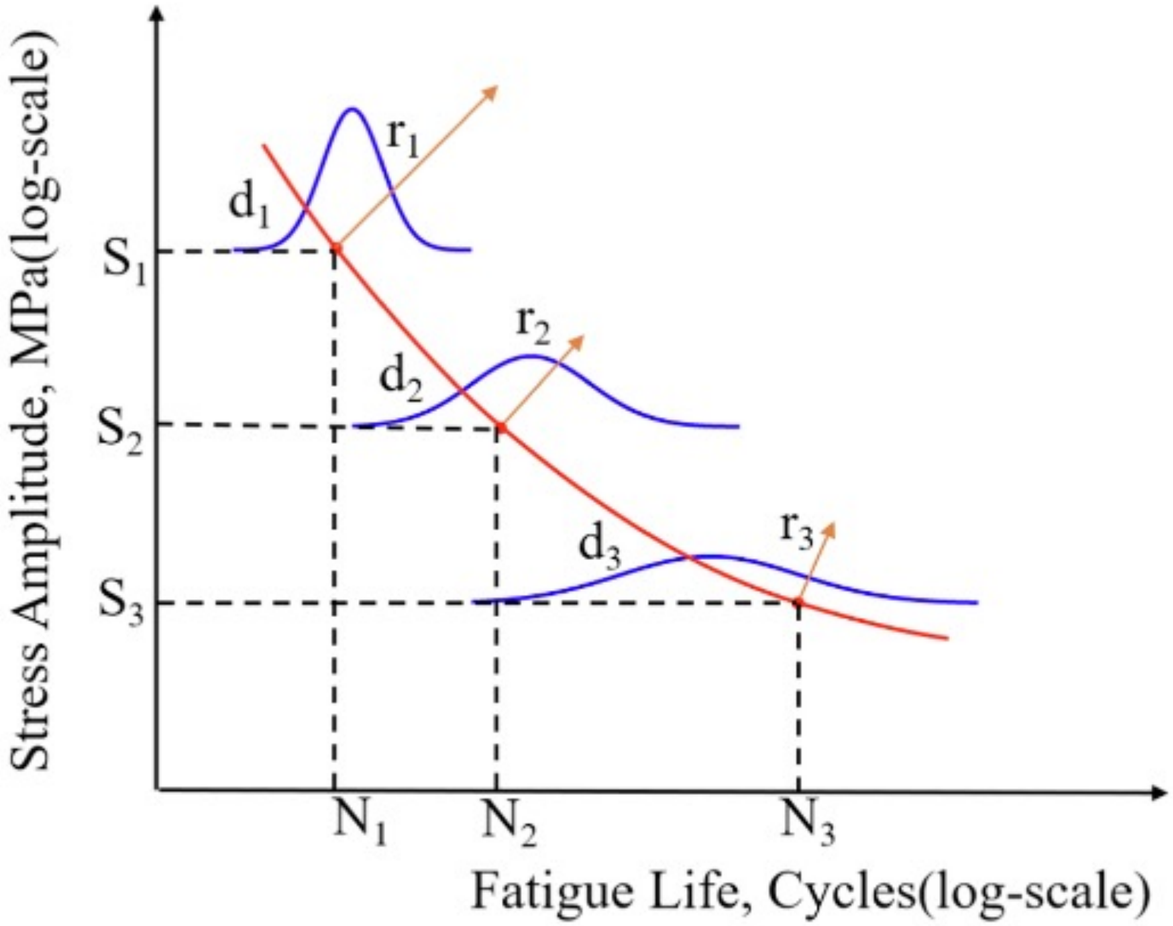


Fig. 1. The schematic diagram of the fatigue probabilistic force-life (P—S—N) curve.

Règles:

- Lorsque la **contrainte diminue**, la durée de **vie moyenne augmente**, N1 < N2 < N3.
- Lorsque **la contrainte diminue**, l'**écart-type** de la durée de vie **augmente,** d1 < d2 < d3
- La **courbure de la courbe S-N diminue** lorsque la **contrainte diminue**, r1 > r2 > r3

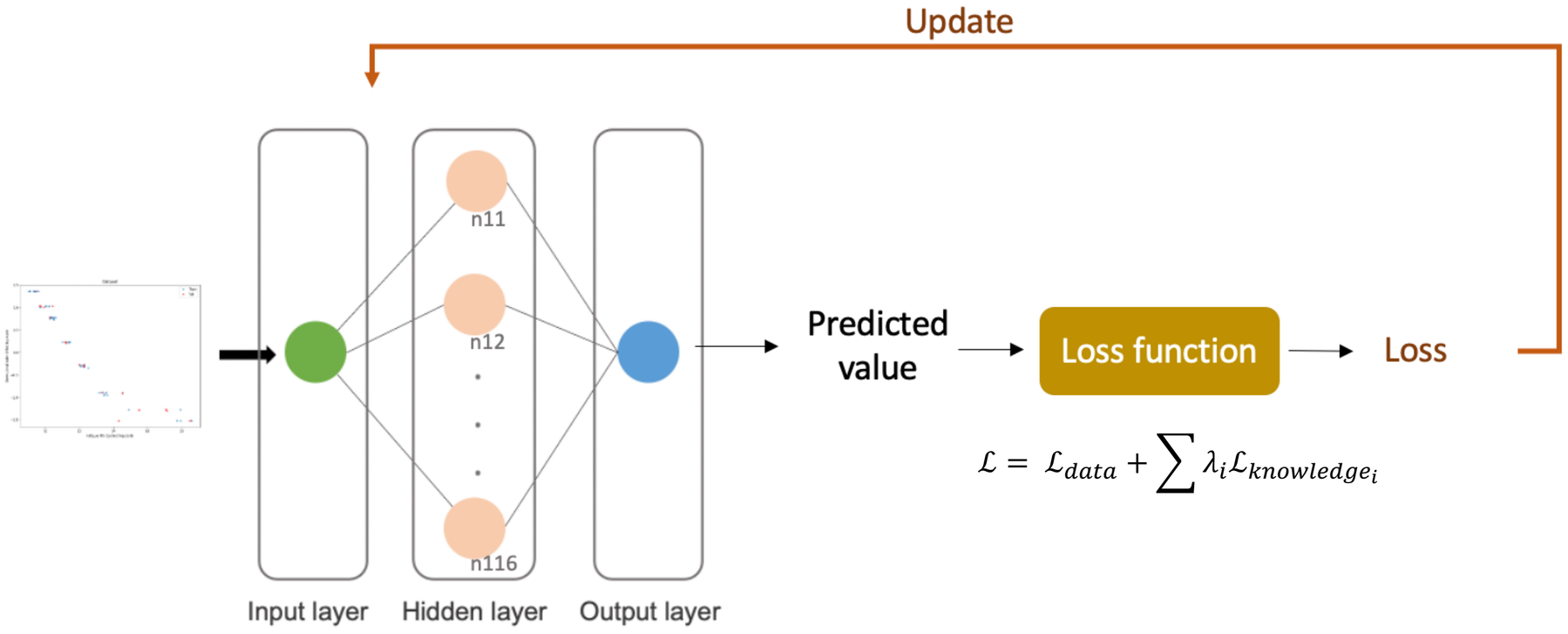
Source: Zhou, T., Jiang, S., Han, T., Zhu, S.-P., & Cai, Y. (2023). A physically consistent framework for fatigue life prediction using probabilistic physics-informed neural network. *International Journal of Fatigue*, *166*, 107234. https://doi.org/10.1016/j.ijfatigue.2022.107234

Connaissances sur la fatigue des matériaux

Description	Règle	Équation	Signification
Lorsque la **contrainte diminue**, la durée de **vie moyenne augmente**	Yμ diminue lorsque la contrainte augmente	$\frac{dY_\mu}{dX} < 0$	La dérivée première de la durée de vie moyenne Yμ est négative
Lorsque **la contrainte diminue**, l' **'écart-type** de la durée de vie **augmente**	Yσ diminue lorsque la contrainte augmente	$\frac{dY_\sigma}{dX} < 0$	La dérivée première de l'écart-type Yσ est négative
La **courbure de la courbe S-N diminue** lorsque la **contrainte diminue**	$\frac{dY_\mu}{dX}$ augmente avec la contrainte	$\frac{d^2Y_\mu}{dX^2} > 0$	La dérivée seconde de la durée de vie moyenne Yμ est positive

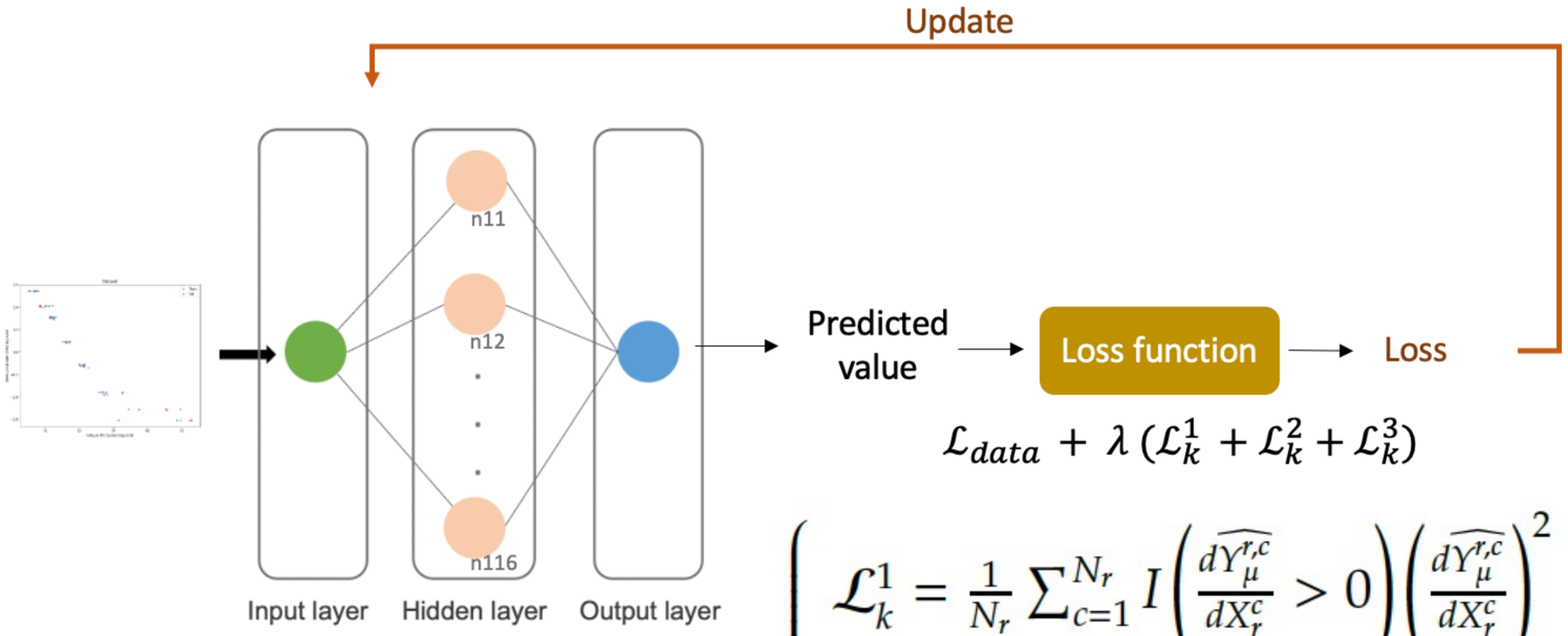
- Yμ: durée de vie moyenne en fatigue
- Yσ: l'écart-type de la durée de vie en fatigue
- X: amplitude de la contrainte

Physics-Informed Neural Network



$$\mathcal{L} = \mathcal{L}_{data} + \sum \lambda_i \mathcal{L}_{knowledge_i}$$

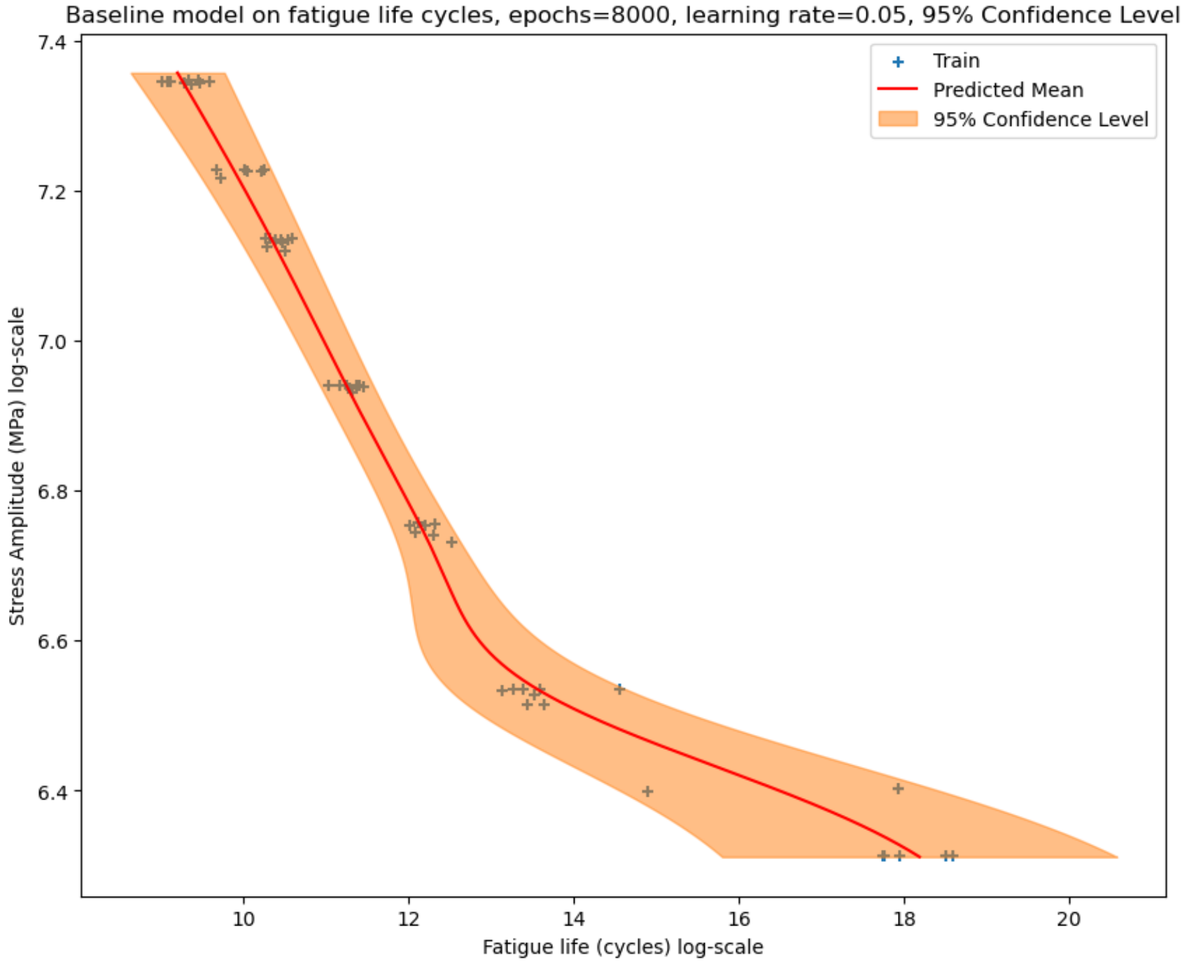
Physics-Informed Neural Network



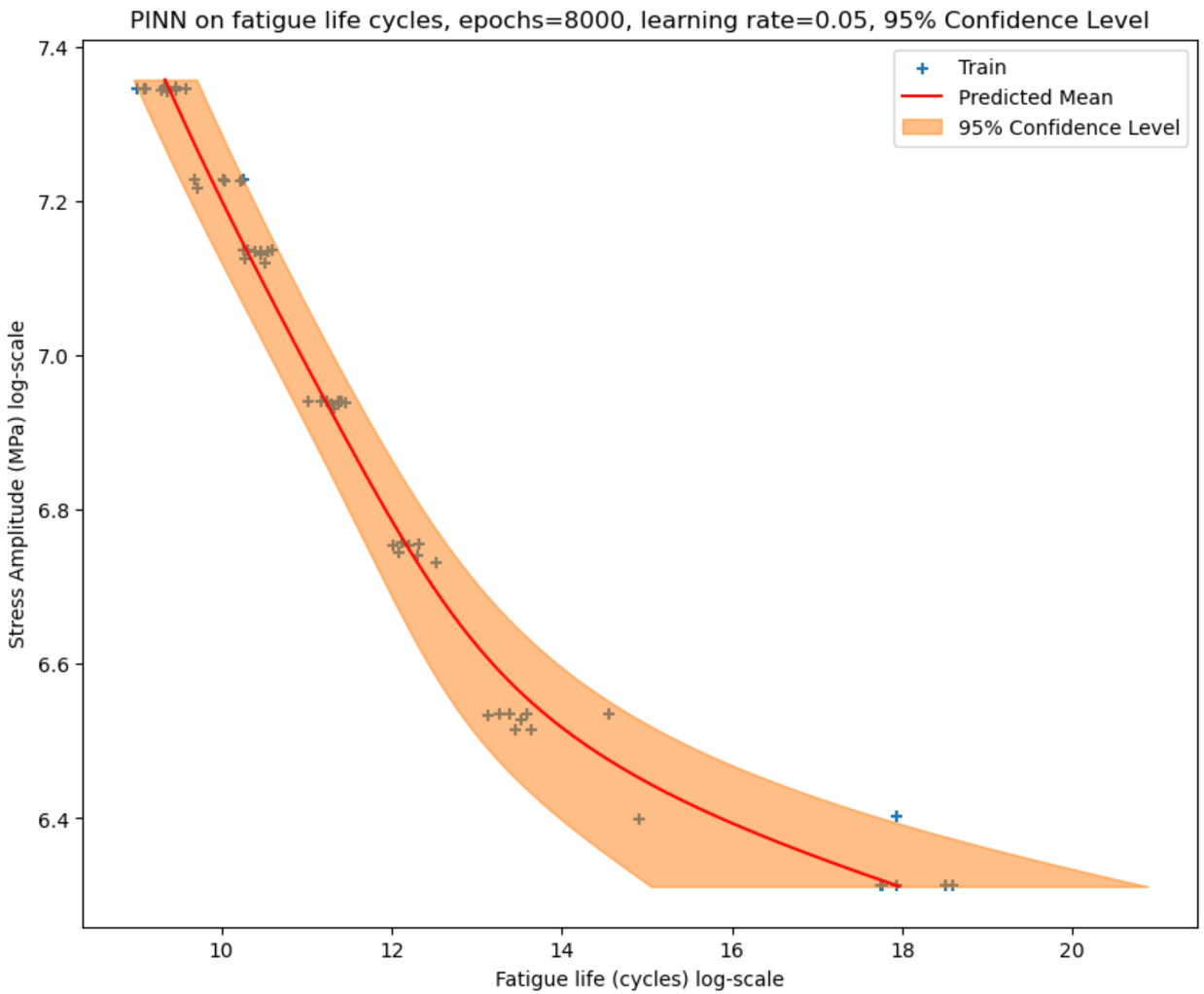
$$\mathcal{L}_{data} + \lambda\left(\mathcal{L}_k^1 + \mathcal{L}_k^2 + \mathcal{L}_k^3\right)$$

$$\begin{cases} \mathcal{L}_k^1 = \frac{1}{N_r}\sum_{c=1}^{N_r} I\left(\frac{d\widehat{Y_\mu^{r,c}}}{dX_r^c} > 0\right)\left(\frac{d\widehat{Y_\mu^{r,c}}}{dX_r^c}\right)^2 \\ \mathcal{L}_k^2 = \frac{1}{N_r}\sum_{c=1}^{N_r} I\left(\frac{d\widehat{Y_\sigma^{r,c}}}{dX_r^c} > 0\right)\left(\frac{d\widehat{Y_\sigma^{r,c}}}{dX_r^c}\right)^2 \\ \mathcal{L}_k^2 = \frac{1}{N_r}\sum_{c=1}^{N_r} I\left(0 > \frac{d^2\widehat{Y_\sigma^{r,c}}}{dX_r^{c2}}\right)\left(\frac{d^2\widehat{Y_\sigma^{r,c}}}{dX_r^{c2}}\right)^2 \end{cases}$$

Le problème de l'évaluation …

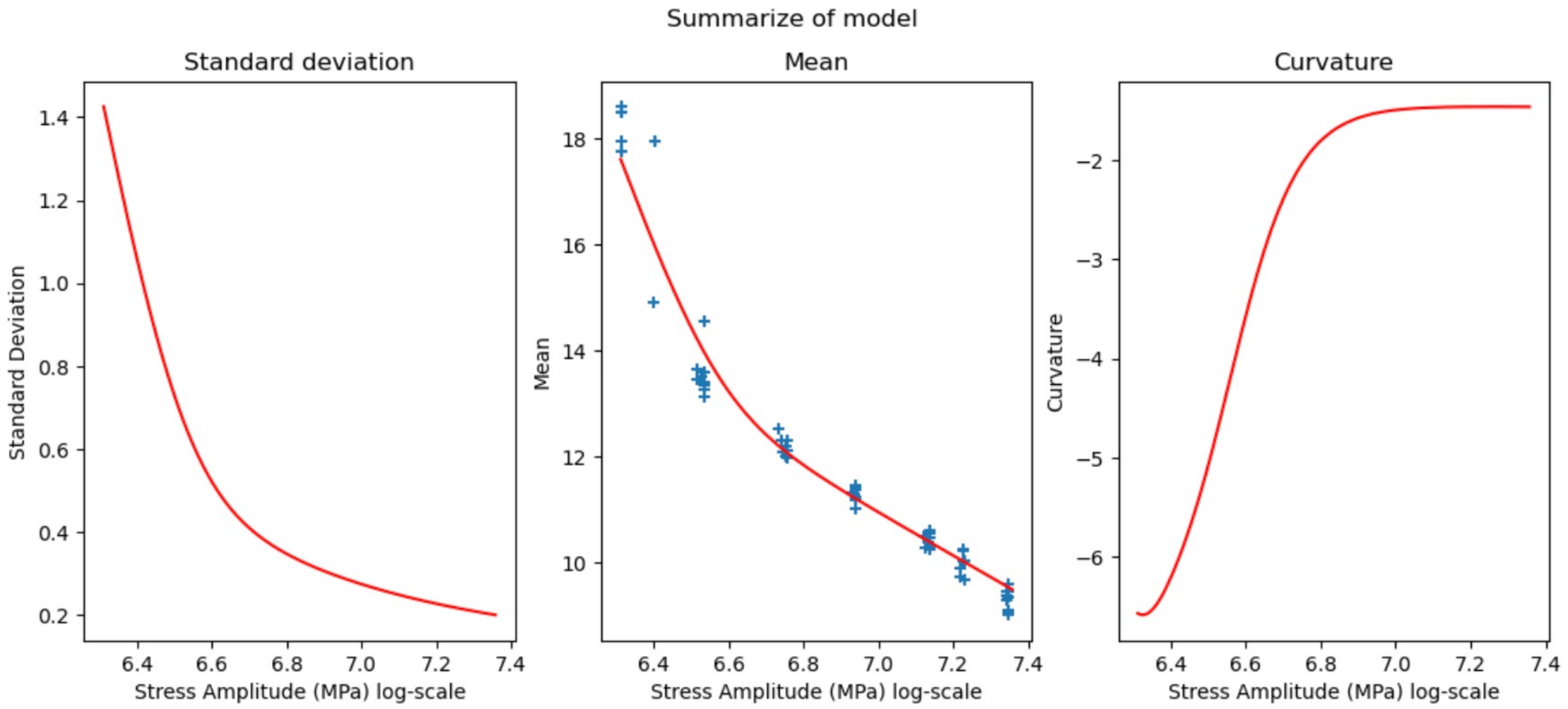


Baseline



PINN

Coefficient de corrélation de Spearman



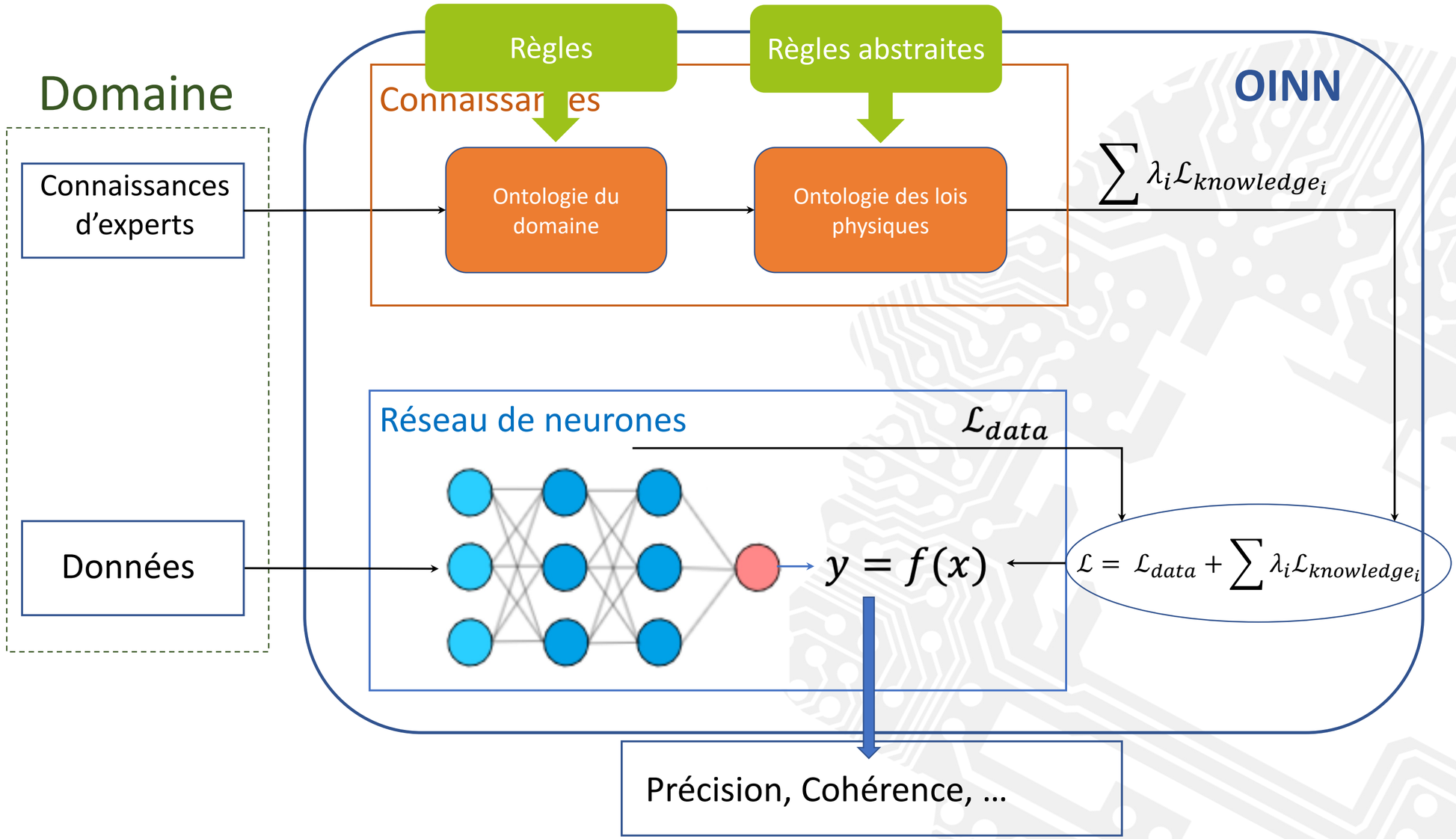
-1 -1 1

Des fonctions monotones …

Règle	Règle abstraite	Équation
Yμ diminue lorsque la contrainte augmente	B diminue quand A augmente	$\frac{dB}{dA} < 0$
Yσ diminue lorsque la contrainte augmente	B diminue quand A augmente	$\frac{dB}{dA} < 0$
$\frac{dY_\mu}{dX}$ augmente avec la contrainte	B augmente quand A augmente	$\frac{dB}{dA} > 0$

- Yμ: durée de vie moyenne en fatigue
- Yσ: l'écart-type de la durée de vie en fatigue
- X: amplitude de la contrainte

Ontology Informed Neural Network



Automating Physical knowledge Integration in Machine Learning. **S. Ghidalia**, O. Labbani Narsis, A. Bertaux and C. Nicolle. 17th IEEE International Conference on Signal Image Technology & Internet-based Systems (SITIS), 2023

Merci pour votre attention

Github

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Bibliographie

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- L. von Rueden *et al.*, “Informed Machine Learning -- A Taxonomy and Survey of Integrating Knowledge into Learning Systems,” *IEEE Trans. Knowl. Data Eng.*, pp. 1–1, 2021, doi: 10.1109/TKDE.2021.3079836.
- J.-X. Wang, J.-L. Wu, and H. Xiao, “A Physics Informed Machine Learning Approach for Reconstructing Reynolds Stress Modeling Discrepancies Based on DNS Data,” *Phys. Rev. Fluids*, vol. 2, no. 3, p. 034603, Mar. 2017, doi: 10.1103/PhysRevFluids.2.034603.
- J. Ling, A. Kurzawski, and J. Templeton, “Reynolds averaged turbulence modelling using deep neural networks with embedded invariance,” *Journal of Fluid Mechanics*, vol. 807, pp. 155–166, Nov. 2016, doi: 10.1017/jfm.2016.615.

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