Symbolic Regression for Turbulent Convection

Predicting Wall Quantities in Rayleigh–Bénard Flows

M1 Mathematics & AI Internship at LISN

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Context - Interpretability

Interpreting Machine Learning models

Its crucial in:

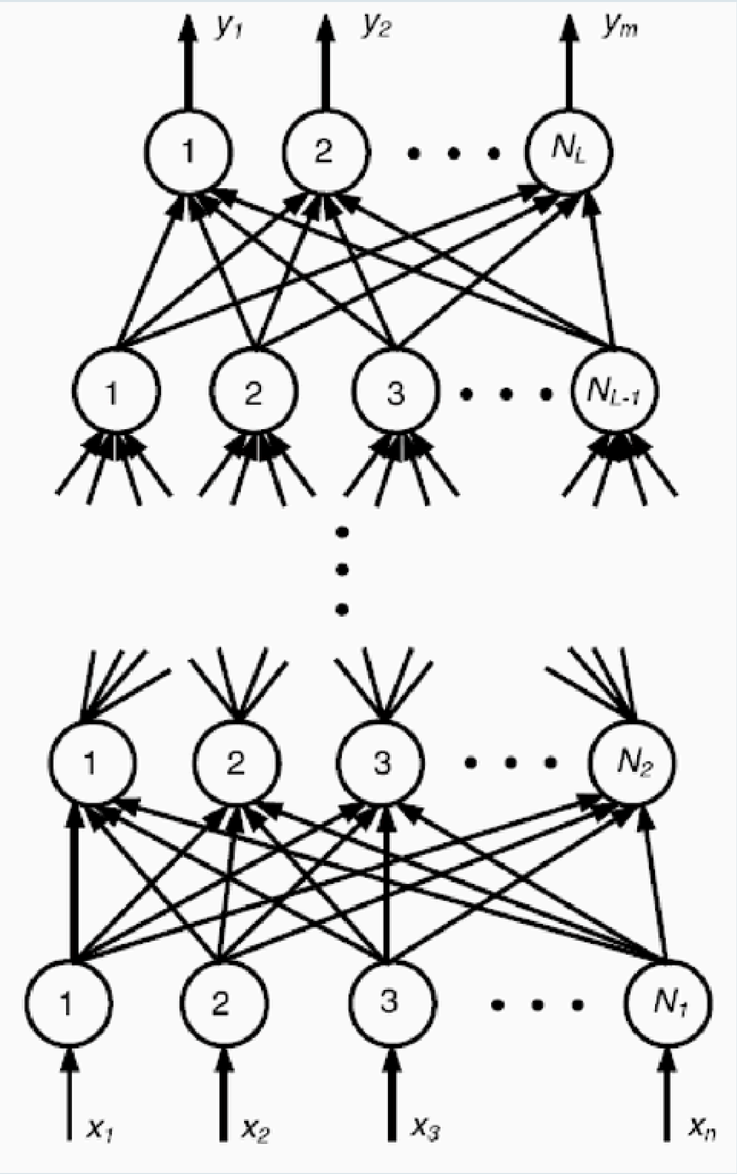
- health
- justice
- engineering
- physics

For example:

- cancer detection
- decision support
- self-driving cars
- discovering physics law from data

eXplainable AI (XAI):

- increasing transparency
- interpret after training
- model intrinsically interpretable



MLP == Black Box ?

Data - Turbulent Convection

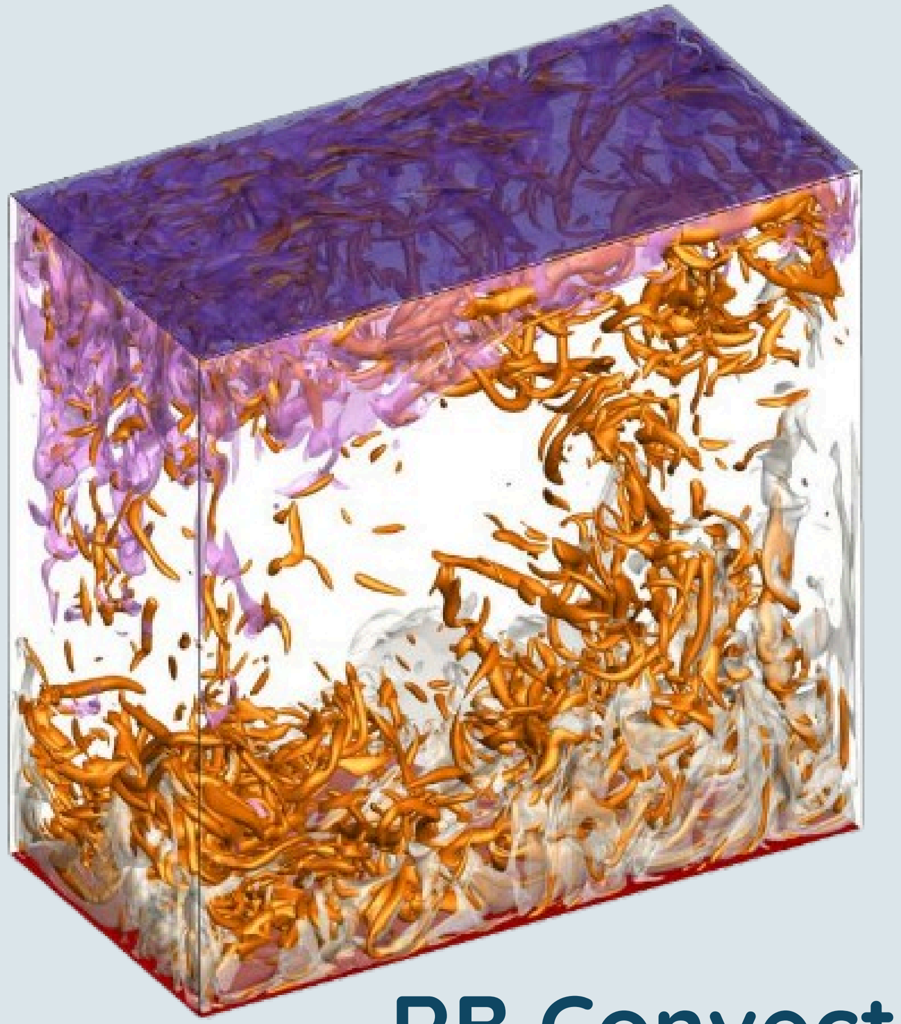
Rayleigh-Bénard Turbulent Convection, suitable data for testing eXplainable AI

Why?

- complex system
- knowed laws
- dominant terms
- non-linearities

Data used:

- Direct Numerical Simulation (DNS)
- turbulence $(\mathrm{Ra} = 2 \cdot 10^9)$
- dimensionless data
- made by COMET team at LISN



RB Convection

Models (could be intrinsically interpretable):

- SINDy (pysindy) [1] - Sparse Identification of Nonlinear Dynamics
- KAN (pykan) [2, 3] - Kolmogorov Arnold Network

Data - Turbulent Convection

(1.1) Incompressibility

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

(1.2) Momentum equation - axis x

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z} = -\frac{\partial p}{\partial x} + \sqrt{\frac{\mathrm{Pr}}{\mathrm{Ra}}}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right)$$

(1.3) Momentum equation - axis y

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z} = -\frac{\partial p}{\partial y} + \sqrt{\frac{\mathrm{Pr}}{\mathrm{Ra}}}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2}\right)$$

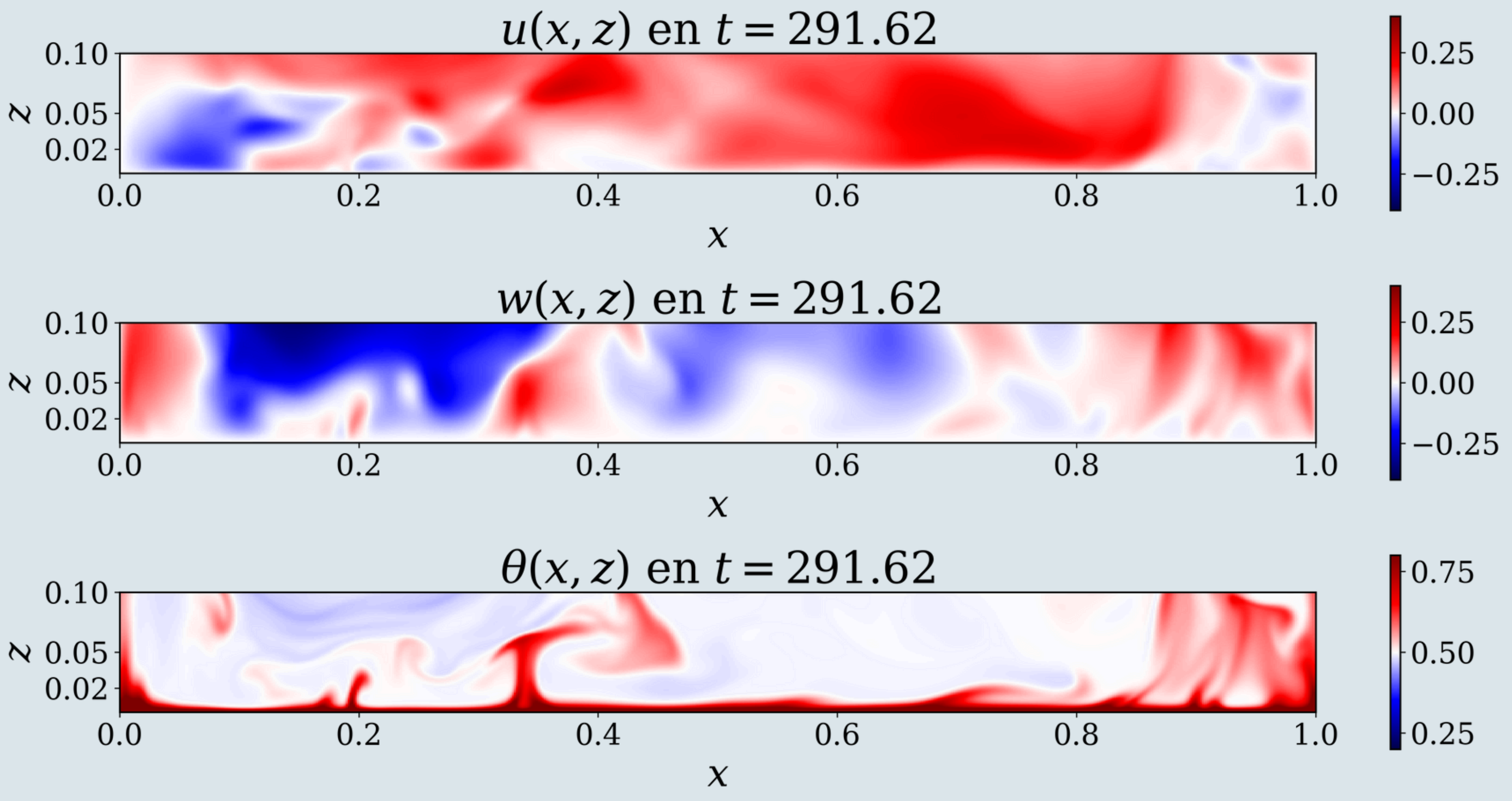
(1.4) Momentum equation - axis z

$$\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial x} + v\frac{\partial w}{\partial y} + w\frac{\partial w}{\partial z} = -\frac{\partial p}{\partial z} + \sqrt{\frac{\mathrm{Pr}}{\mathrm{Ra}}}\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2}\right) + \theta$$

(1.5) Heat transfer equation

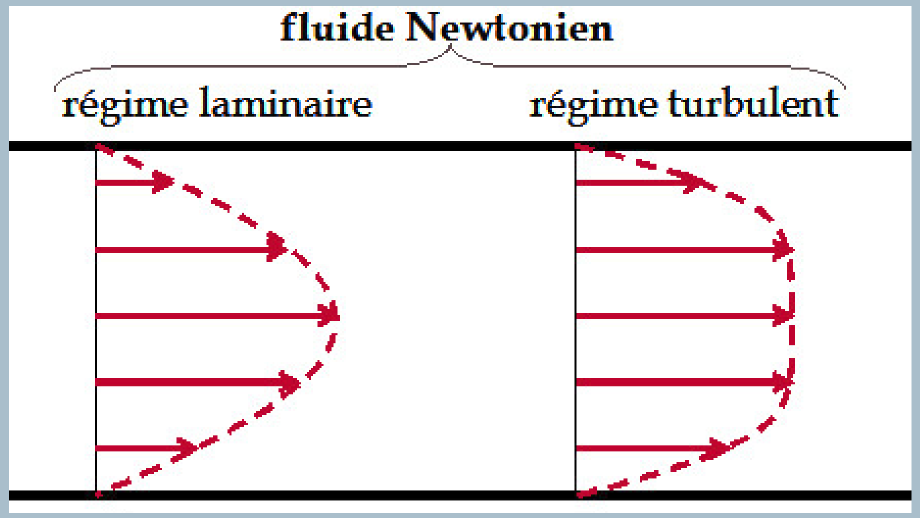
$$\frac{\partial \theta}{\partial t} + u\frac{\partial \theta}{\partial x} + v\frac{\partial \theta}{\partial y} + w\frac{\partial \theta}{\partial z} = \sqrt{\frac{1}{\mathrm{Pr}\cdot\mathrm{Ra}}}\left(\frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2} + \frac{\partial^2 \theta}{\partial z^2}\right)$$

Navier-Stokes Equations



Speeds and temperature profiles

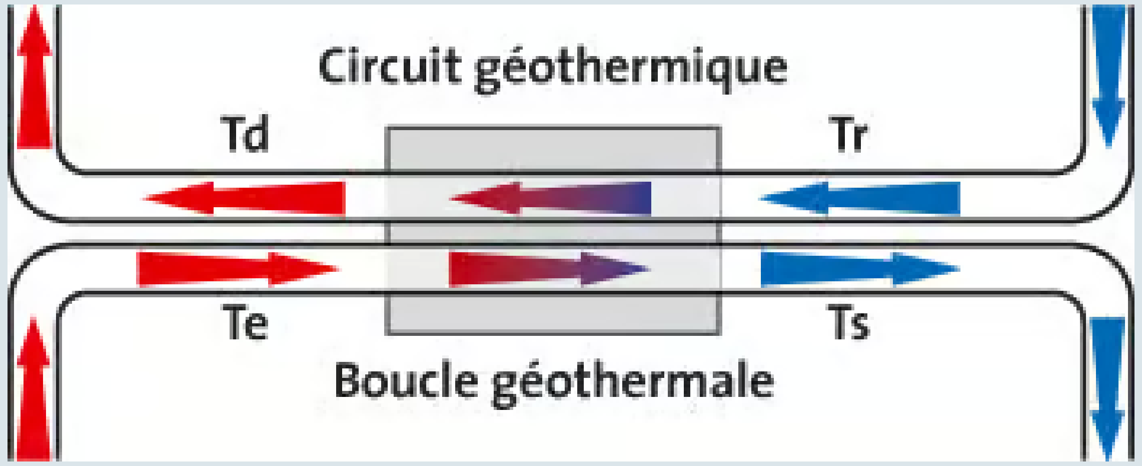
Objectives - Wall Laws



Wall shear stress

$$\tau = \mu \frac{\partial u}{\partial z}\bigg|_{z=0}$$

Loss of fluid speed due to viscous friction



Wall heat flux

$$q = -k \frac{\partial \theta}{\partial z}\bigg|_{z=0}$$

Heat exchange between the wall and the fluid

It is studied in:

- aeronautics (plane wings)
- geodynamics (earthquake)

It is studied in:

- energy (energy efficiency)
- engineering (data center cooling)

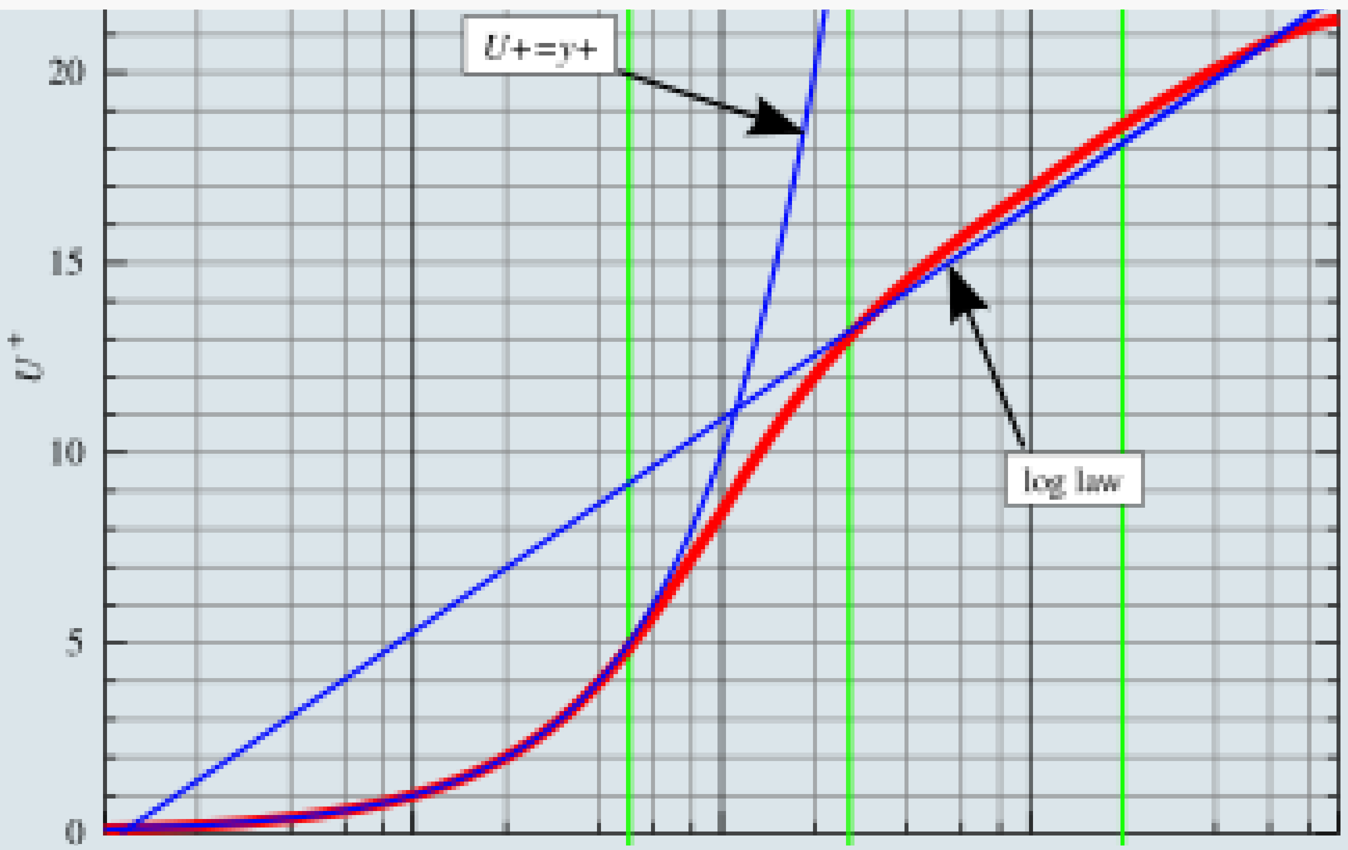
Objective - Wall Laws

Problematic

- viscous sublayer (near wall) is very thin and follows a specific dynamic
- simulations are computationally expensive => often low-resolved
- experimentally inaccessible (sensors disrupt dynamics)

$$\tau = \mu \frac{\partial u}{\partial z}\bigg|_{z=0} \qquad q = -k \frac{\partial \theta}{\partial z}\bigg|_{z=0}$$

Cannot be derived



Wall laws: flow regime

Can we find equations to get these values with low-resolution data?

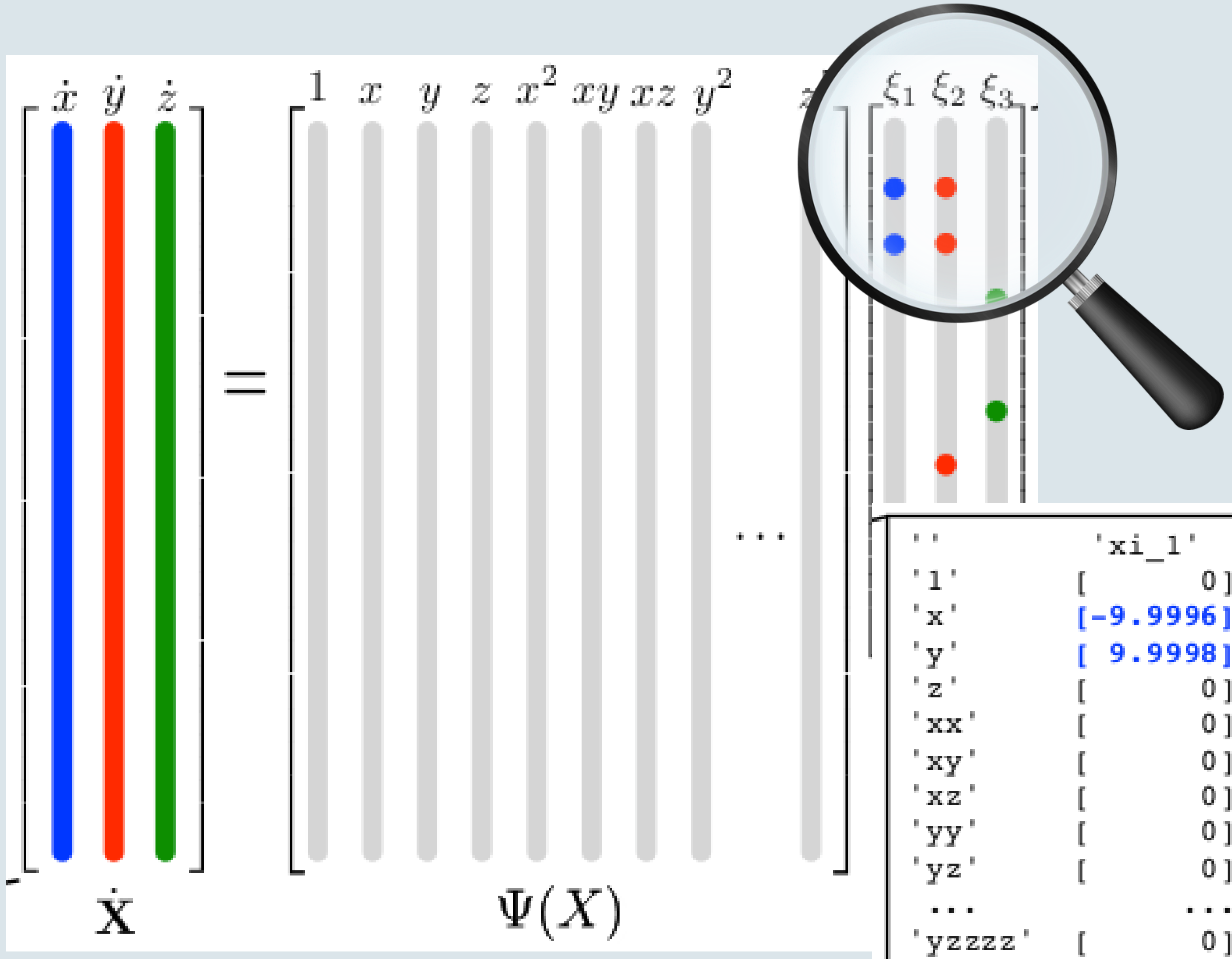
Methodology: Predicting a symbolic equation of field $\frac{\partial u}{\partial z}$ and $\frac{\partial \theta}{\partial z}$ on a restricted vertical plane

Sparse Identification of Nonlinear Dynamics (SINDy)

System representation:

$$\dot{X} = \Psi(X)\Xi + \varepsilon$$

- **<u>Idea:</u>** A few terms dominate dynamic systems
- Library of nonlinear functions $\Psi(X)$
- LASSO regression for parsimony: $\|\Xi\|_1 = \sum_i^p |\xi_i|$



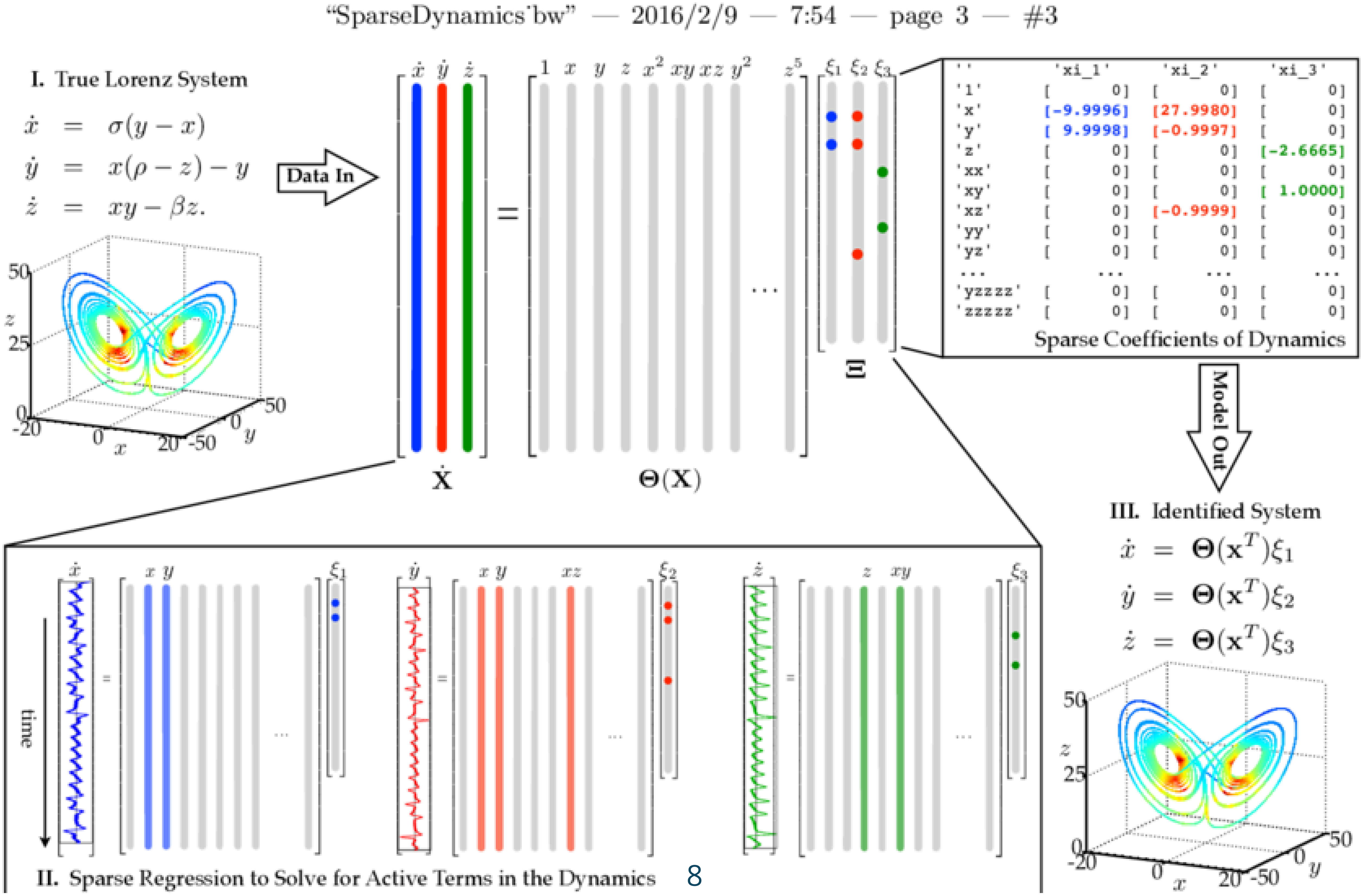
''	'xi_1'	'xi_2'	'xi_3'
'1'	[0]	[0]	[0]
'x'	[-9.9996]	[27.9980]	[0]
'y'	[9.9998]	[-0.9997]	[0]
'z'	[0]	[0]	[-2.6665]
'xx'	[0]	[0]	[0]
'xy'	[0]	[0]	[1.0000]
'xz'	[0]	[-0.9999]	[0]
'yy'	[0]	[0]	[0]
'yz'	[0]	[0]	[0]
...	...	...	...
'yzzzz'	[0]	[0]	[0]
'zzzzz'	[0]	[0]	[0]

Sparse Coefficients of Dynamics

Ξ

<u>Loss function:</u> $$\arg\min_{\Xi} ||\Psi(X)\Xi - \dot{X}||_2^2 + \lambda||\Xi||_1$$

Sparse Identification of Nonlinear Dynamics (SINDy)



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'yy'	[0]	[0]	[0]
'yz'	[0]	[0]	[0]
...	...	...	...
'yzzzz'	[0]	[0]	[0]
'zzzzz'	[0]	[0]	[0]

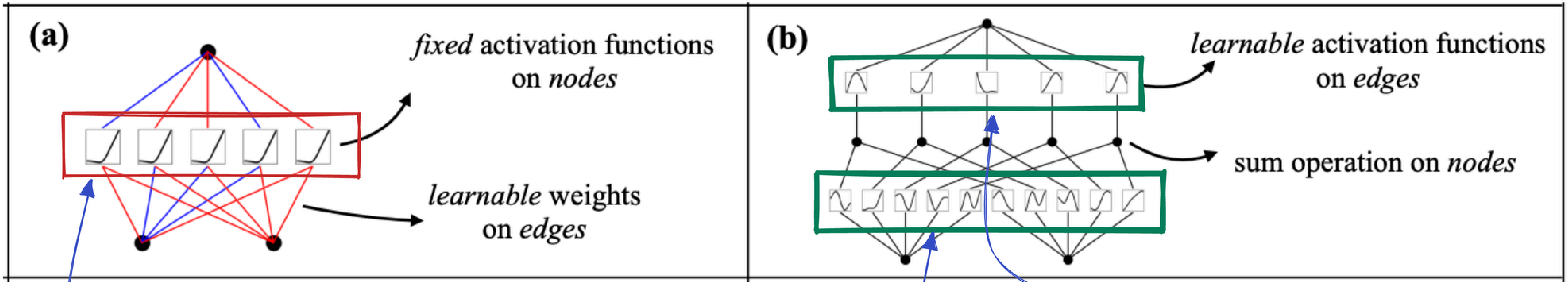
Kolmogorov Arnold Network (KAN)

Neural Network

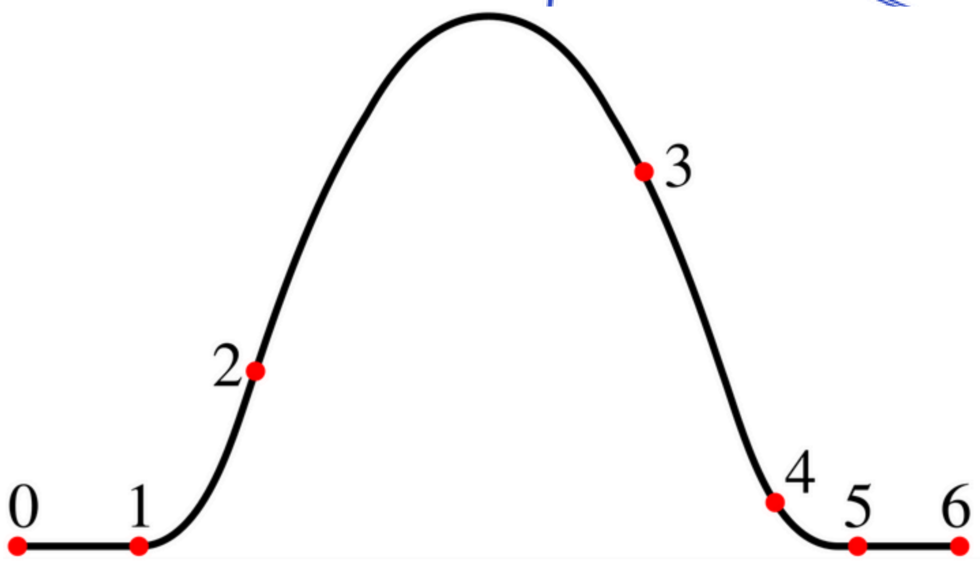
Universal approximation theorem

KAN

Kolmogorov-Arnold representation theorem



All neurons have
a fixed activation
function



Every edge has
a different
activation
function
learned with splines

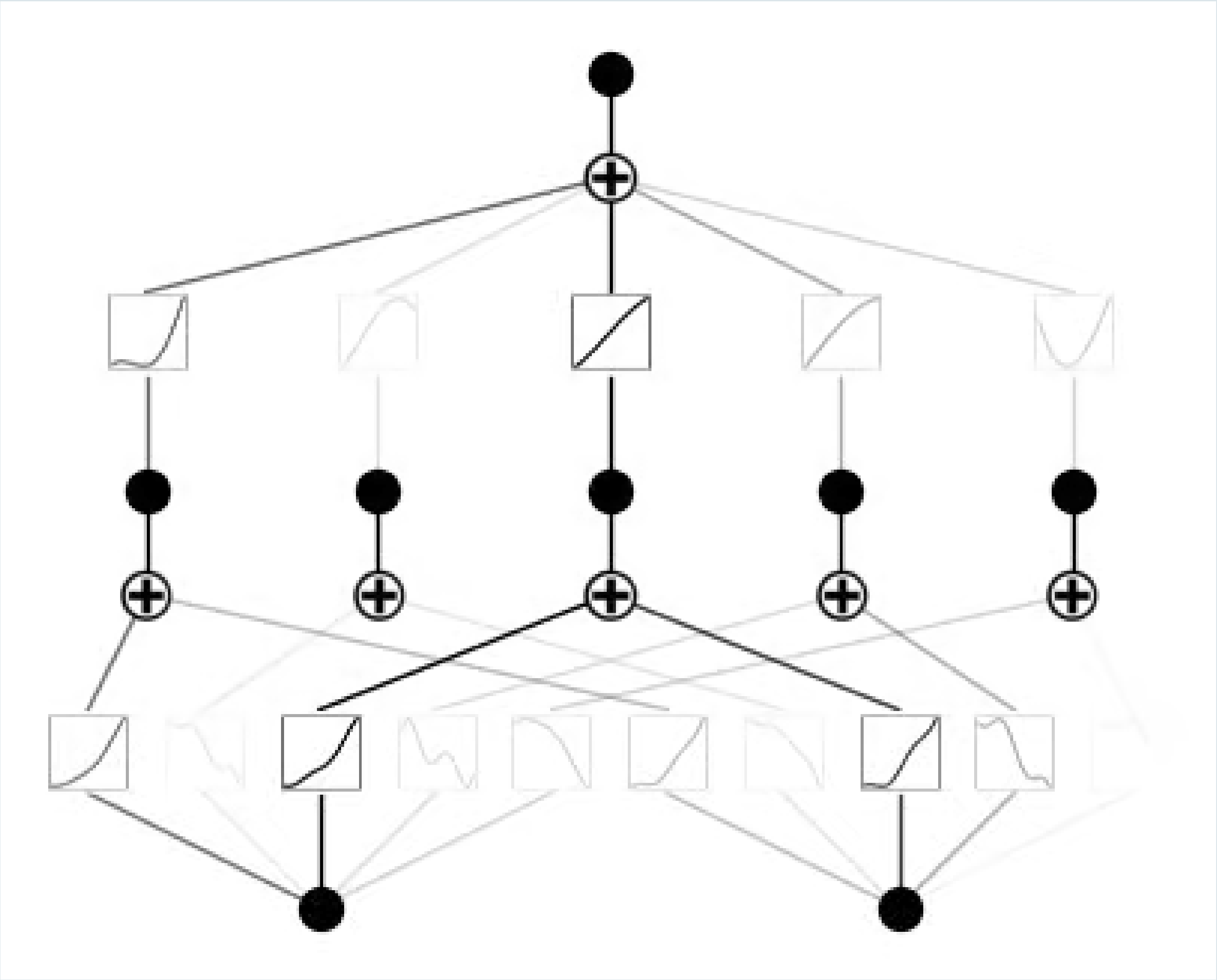
Kolmogorov Arnold Network (KAN)

<u>**Advantages:**</u>

- According to the litterature: KANs are **as good or better** than MLPs
- WITH a network **less deep** and **less wide**
- AND we can use **pruning**
- SO it is **EASIER TO INTERPRET**

<u>**MORE THAN THAT:**</u>

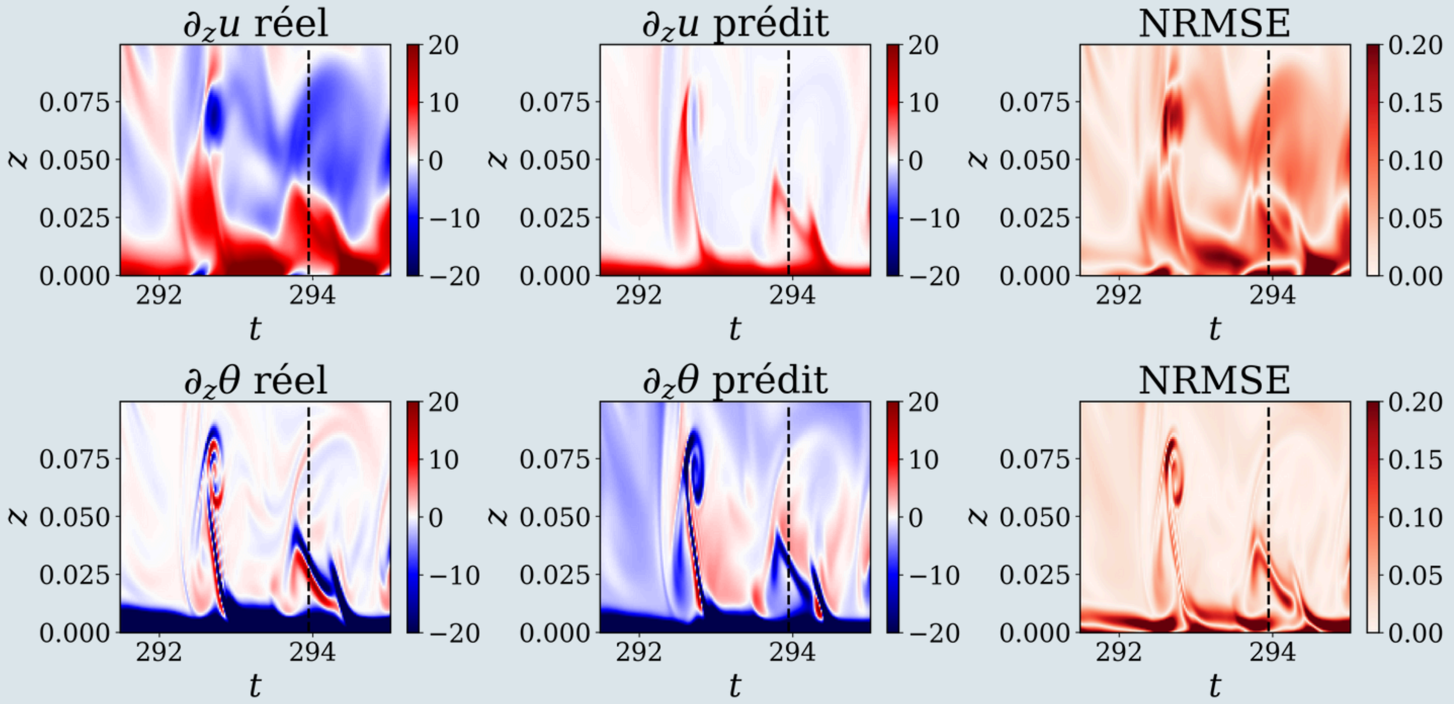
- Transform spline activation into symbolic expression with symbolic regression methods
- We can extract symbolic expression as SINDy



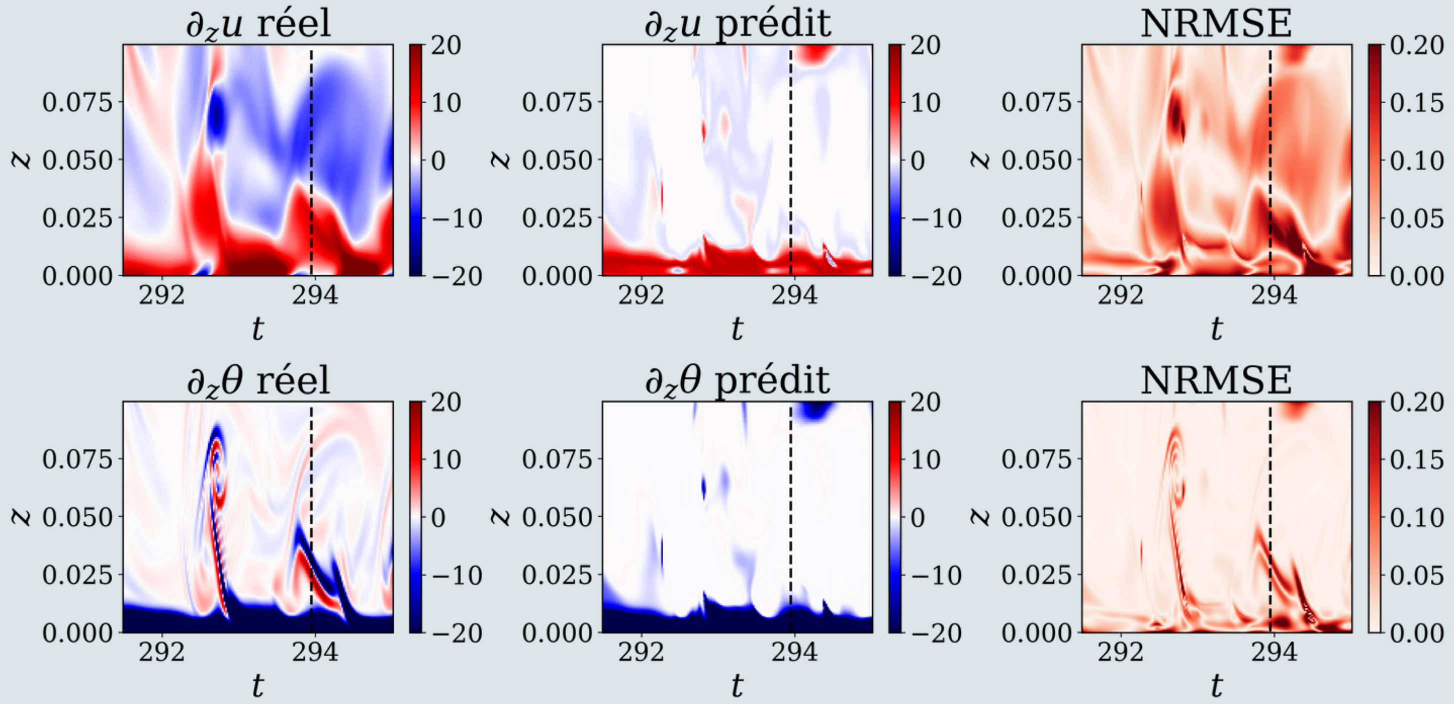
Pruning a KAN

Estimation of $\dfrac{\partial(u,\theta)}{\partial z}$ on the (z,t) plane

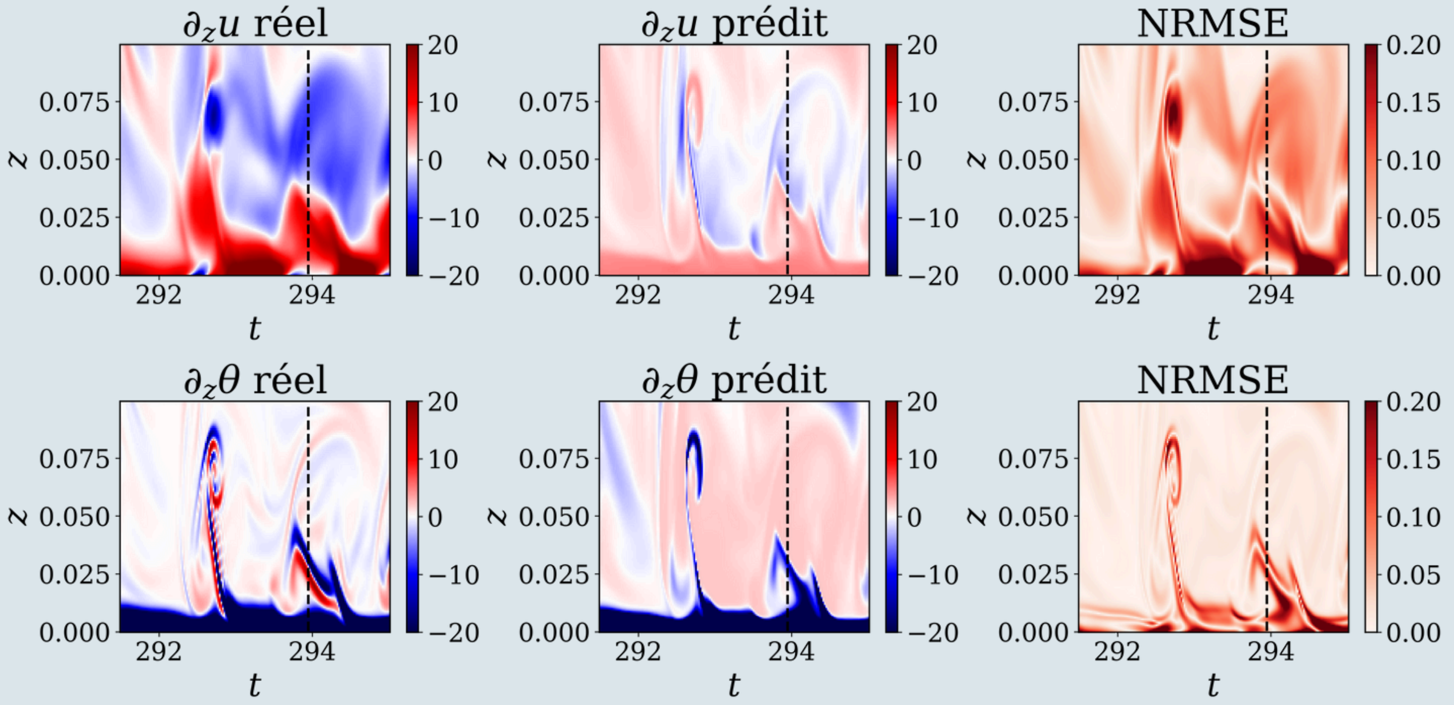
SINDy



KAN



S-KAN



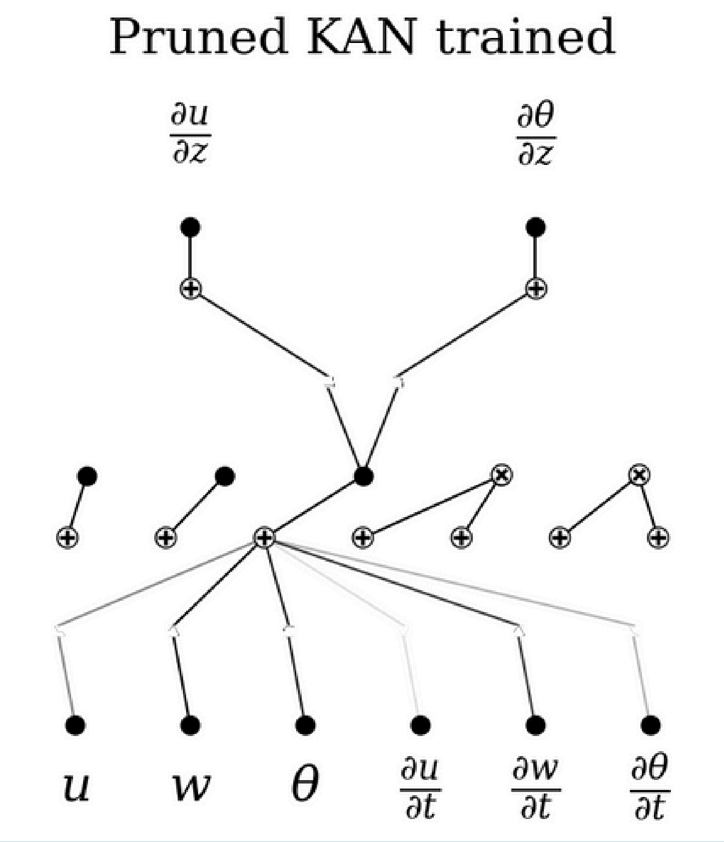
Model	SINDy	KAN	S-KAN
RMSE	*8.519*	*8.330*	*8.507*
R^2	*0.724*	*0.751*	*0.740*

Estimation of $\frac{\partial(u,\theta)}{\partial z}$ *on the* (z,t) *plane*

SINDy

$$
\begin{cases}
\dfrac{\partial u}{\partial z} = -19.381 + 39.741\,\theta - 12.377\,\dfrac{\partial w}{\partial t} + 27.052\,w\dfrac{\partial \theta}{\partial t} \\[2ex]
\dfrac{\partial \theta}{\partial z} = 83.216 + 15.150\,u - 177.133\,\theta - 74.524\,\dfrac{\partial u}{\partial t} \\[2ex]
\qquad -5.864\,\dfrac{\partial \theta}{\partial t} + 153.060\,u\dfrac{\partial \theta}{\partial t} + 19.903\,\theta\dfrac{\partial \theta}{\partial t}
\end{cases}
$$

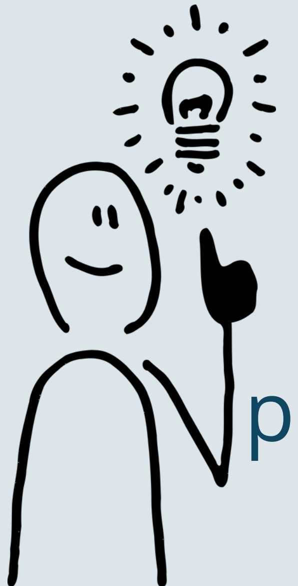
KAN



1. Similar performance but KAN performs better
2. SINDy is more interpretable
3. Concentrated errors close to the wall

S-KAN

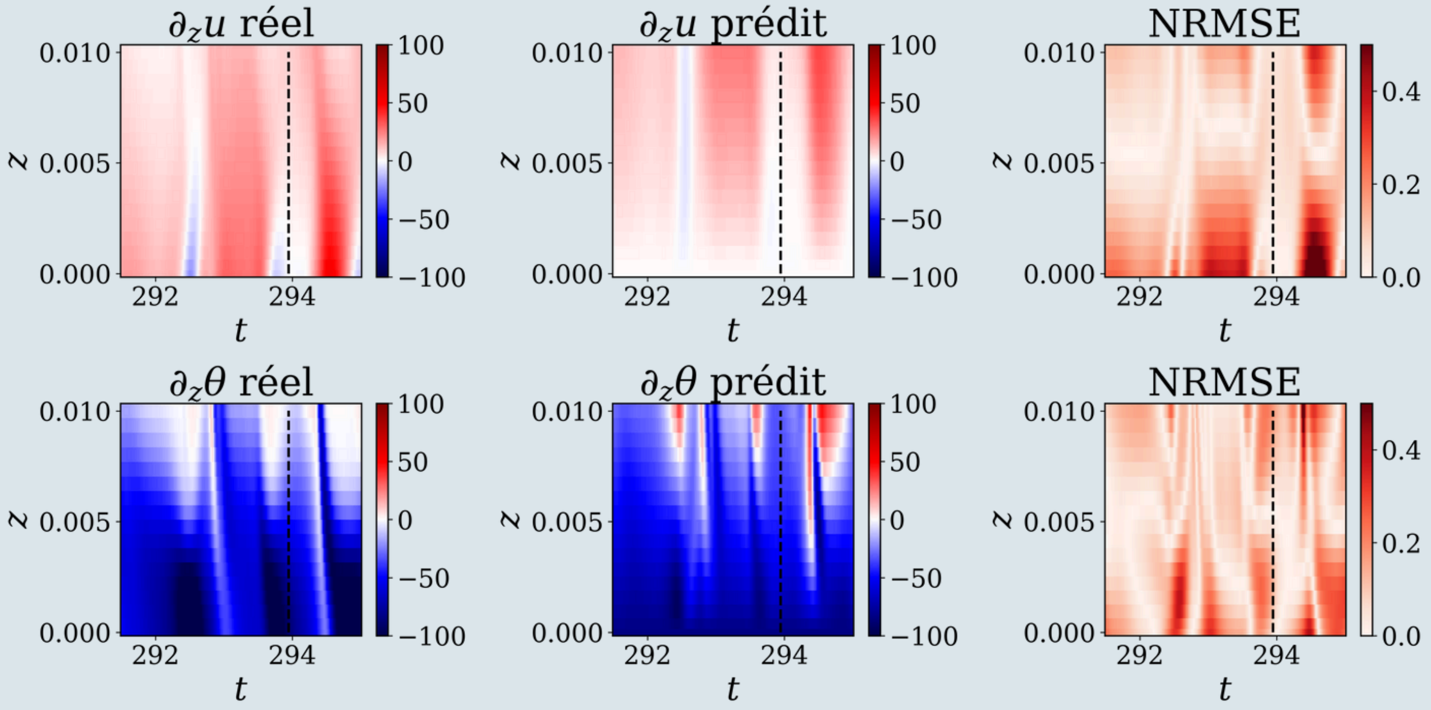
$$
\begin{cases}
\dfrac{\partial u}{\partial z} = 6.027 - 0.795\,u - 0.314\,w - 2.387\,\exp\left(-2.522\,\theta\right) \\
\qquad -0.165\,\dfrac{\partial u}{\partial t} - 0.210\left(-\dfrac{\partial w}{\partial t} - 0.382\right)^2 - 0.246\,\dfrac{\partial \theta}{\partial t} \\[2ex]
\dfrac{\partial \theta}{\partial t} = 2.833 - 44.755\,\exp\left[-0.458\,u - 0.181\,w - 1.374\,\exp\left(-2.522\,\theta\right)\right] \\
\qquad \times \exp\left[-0.095\,\dfrac{\partial u}{\partial t} - 0.121\left(-\dfrac{\partial w}{\partial t} - 0.382\right)^2 - 0.142\,\dfrac{\partial \theta}{\partial t}\right]
\end{cases}
$$



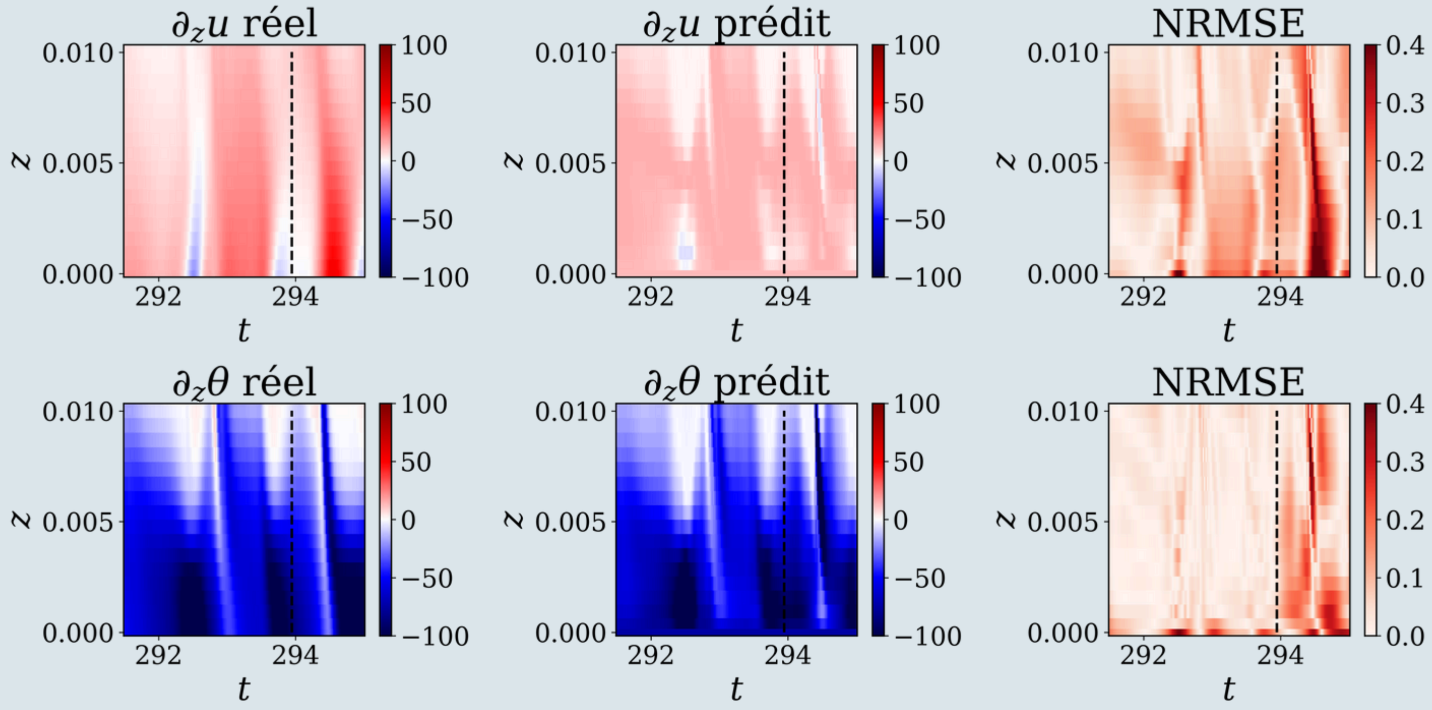
Improve near-wall performance

Estimation of $\frac{\partial(u,\theta)}{\partial z}$ *in the viscous sublayer* $z < 0.01$

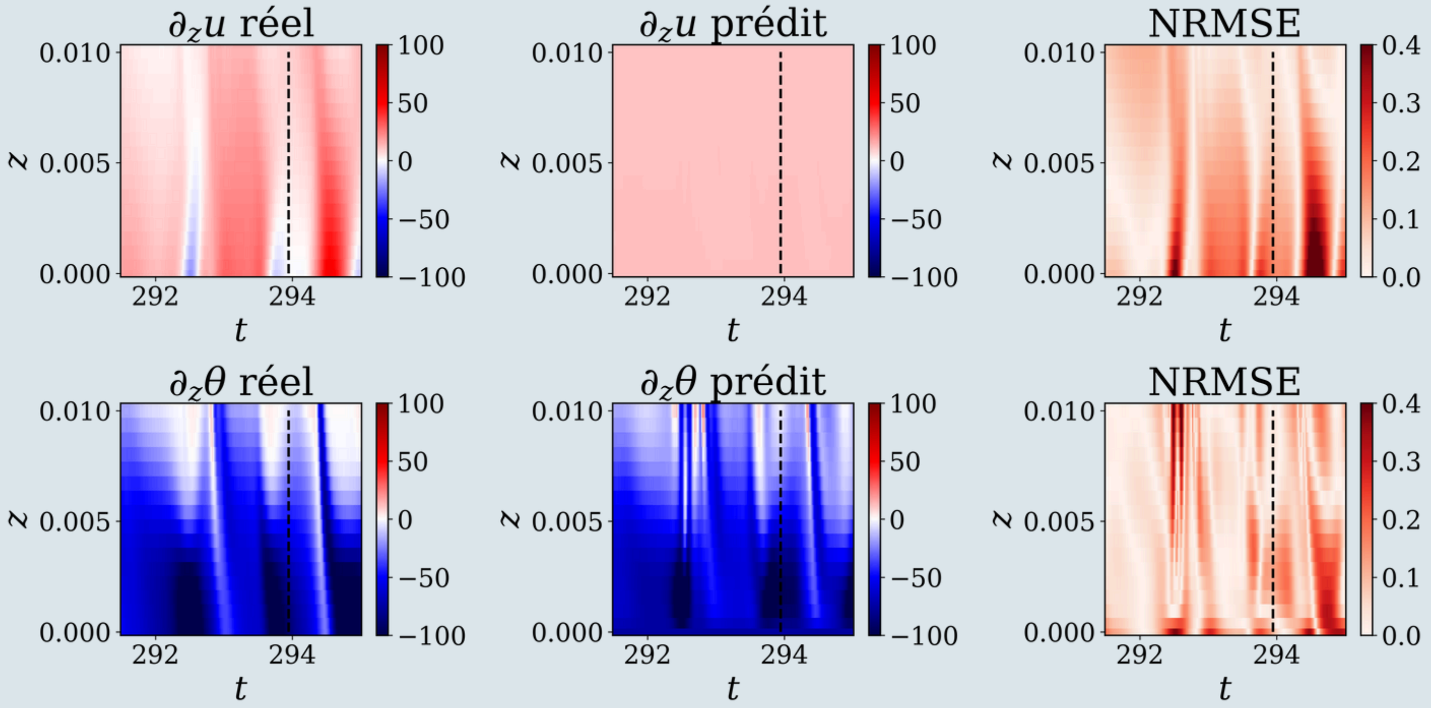
SINDy



KAN



S-KAN



Model	SINDy	KAN	S-KAN
RMSE	*18.663*	*16.909*	*16.209*
R^2	*0.527*	*0.612*	*0.644*

Estimation of $\frac{\partial(u,\theta)}{\partial z}$ *in the viscous sublayer* $z < 0.01$

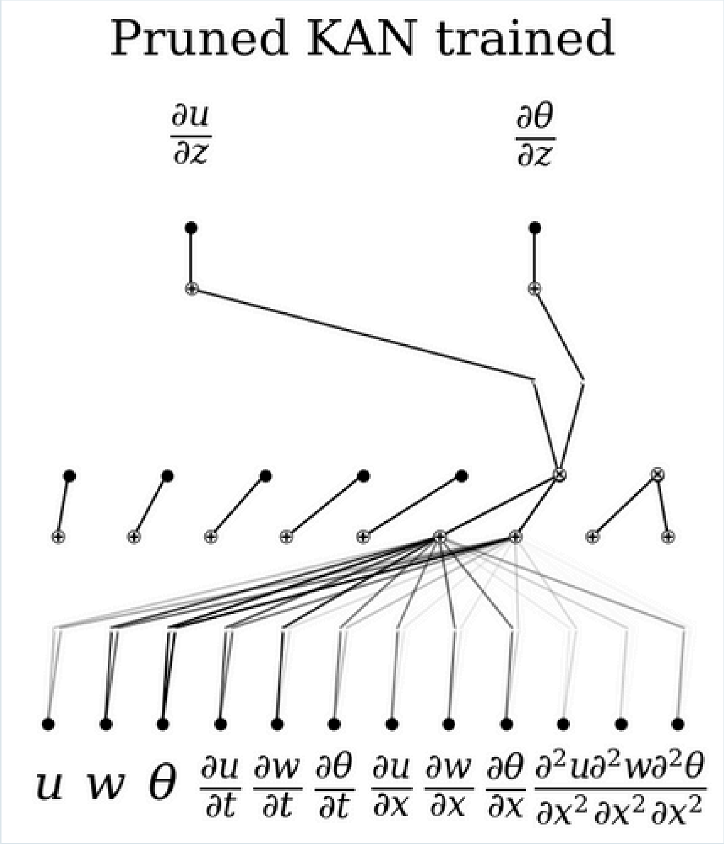
SINDy

$$\begin{cases} \dfrac{\partial u}{\partial z} = & 120.350\,u \\ \dfrac{\partial \theta}{\partial z} = & 140.430\,u - 1041.069\,w - 83.790\,\theta + 22.008\dfrac{\partial u}{\partial t} - 45.874\,u\dfrac{\partial \theta}{\partial t} \\ & -35.446\,w\dfrac{\partial w}{\partial t} + 68.847\,\theta\dfrac{\partial u}{\partial t} - 106.329\,u\dfrac{\partial w}{\partial x} - 14.933\,u\dfrac{\partial \theta}{\partial x} \\ & +72.401\,w\dfrac{\partial u}{\partial x} - 8.799\,w\dfrac{\partial \theta}{\partial x} - 17.126\,\theta\dfrac{\partial u}{\partial x} + 126.378\,\theta\dfrac{\partial w}{\partial x} \end{cases}$$

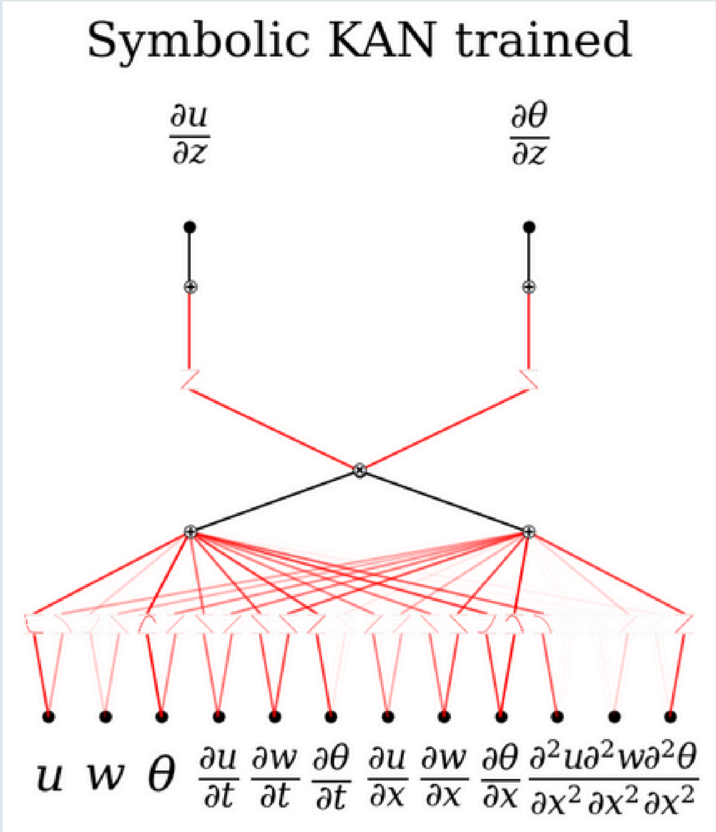
Momentum transport

Heat transfer

KAN



S-KAN



1. Better performance for S-KAN
2. SINDy remains more interpretable
3. Specializing models is a good idea

Conclusion and future work

Conclusion:

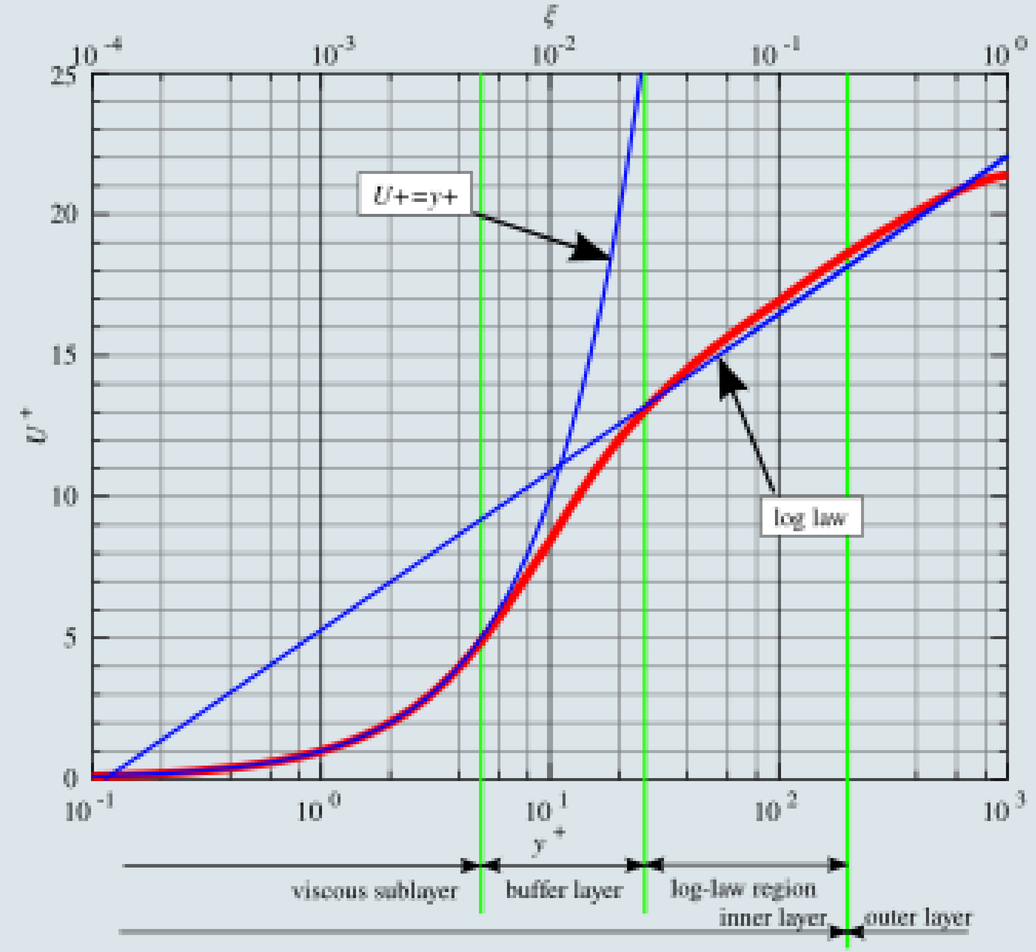
- It is possible to extract reduced equations from the dynamic system based on simulation data.

Both approaches are promising.

- For SINDy, use is limited (prediction of continuous fields only) but more interpretable.
- KANs are more flexible and could lead to better results with other uses.

Future work:

- Try ensemble models or combine expert models: train expert models according to layer (viscous, connection, logarithmic, external) and then assemble them to predict fields
- Try to predict directly at the wall with low-resolution data



Wall laws: flow regime

Thank you for listening

Key references:

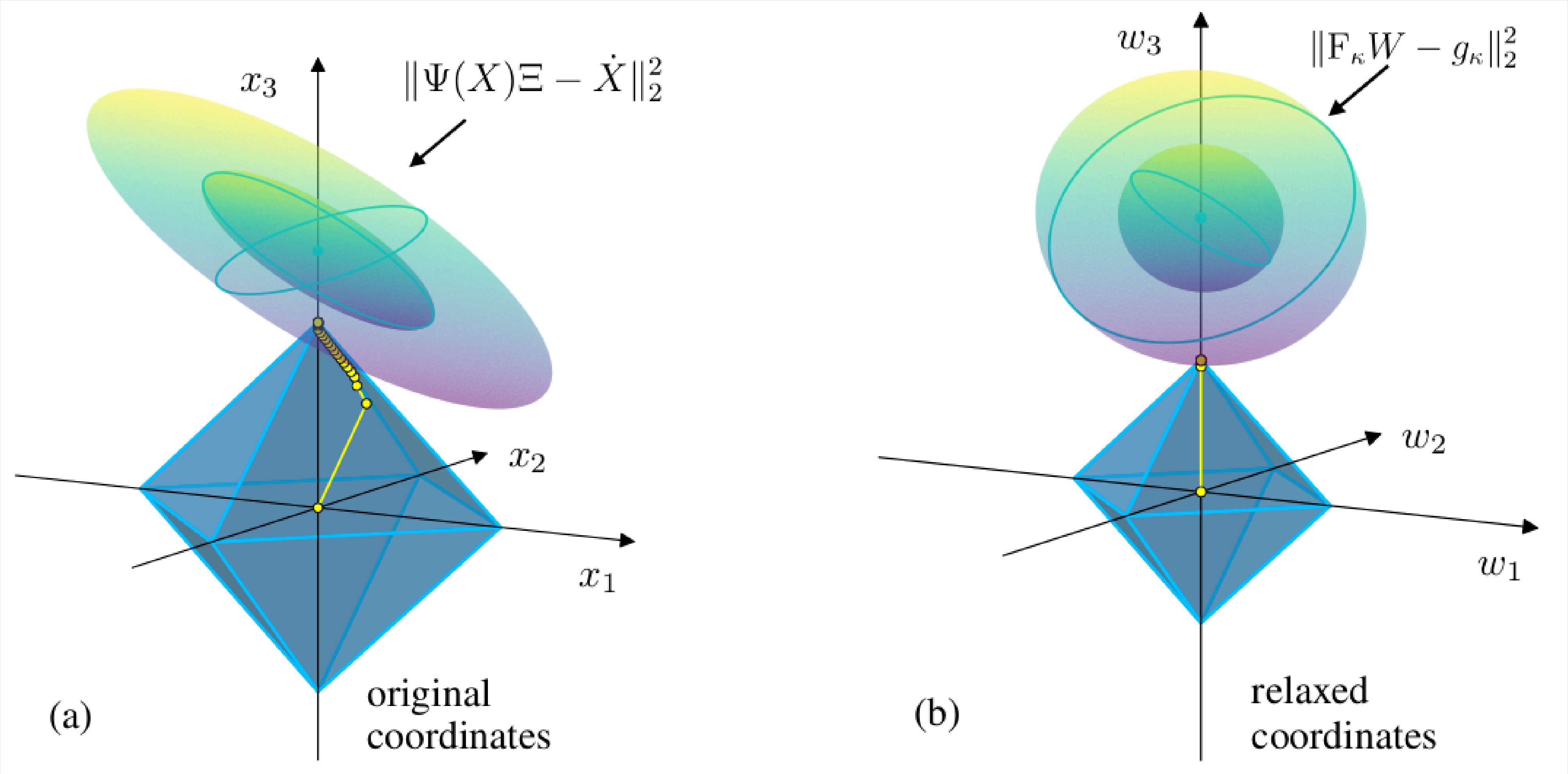
- [1] Brunton, S. L., Proctor, J. L., & Kutz, J. N. (2015). Discovering governing equations from data : Sparse identification of nonlinear dynamical systems (No. arXiv:1509.03580). arXiv. https://doi.org/10.48550/arXiv.1509.03580
- [2] Liu, Z., Wang, Y., Vaidya, S., Ruehle, F., Halverson, J., Soljačić, M., Hou, T. Y., & Tegmark, M. (2025). Kan : Kolmogorov-arnold networks (No. arXiv:2404.19756). arXiv. https://doi.org/10.48550/arXiv.2404.19756
- [3] Liu, Z., Ma, P., Wang, Y., Matusik, W., & Tegmark, M. (2024). Kan 2. 0 : Kolmogorov-arnold networks meet science (No. arXiv:2408.10205). arXiv. https://doi.org/10.48550/arXiv.2408.10205

Optimization : SR3

$$\arg\min_{\Xi} ||\Psi(X)\Xi - \dot{X}||_2^2 + \lambda R(W) + \frac{\kappa}{2}||\Xi - W||_2^2$$

- Break the problem down into two parts:
  - The reconstruction error for Ξ
  - Regularization for W
- Faster optimization due to better conditioning:

$$\mathrm{cond}(\mathrm{F}_\kappa) = \mathrm{cond}(\Psi(X))\sqrt{\frac{\kappa + \sigma_{\min}(\Psi(X))^2}{\kappa + \sigma_{\max}(\Psi(X))^2}}$$



Partial minimization:

$$\Xi^*(W) = H_\kappa^{-1}(\Psi(X)^T\dot{X} + \kappa W)$$

Final minimization:

$$W^* = \arg\min_{W} \frac{1}{2}||\mathrm{F}_\kappa W - g_\kappa||_2^2 + \lambda R(W)$$

$$\mathrm{F}_\kappa = \begin{bmatrix} \kappa\Psi(X)H_\kappa^{-1} \\ \sqrt{\kappa}(I_p - \kappa H_\kappa^{-1}) \end{bmatrix}, \quad g_\kappa = \begin{bmatrix} I_p - \Psi(X)H_\kappa^{-1}\Psi(X)^T \\ \sqrt{\kappa}H_\kappa^{-1} \end{bmatrix}\dot{X}$$