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# META MODELLING / HYBRID MODELLING

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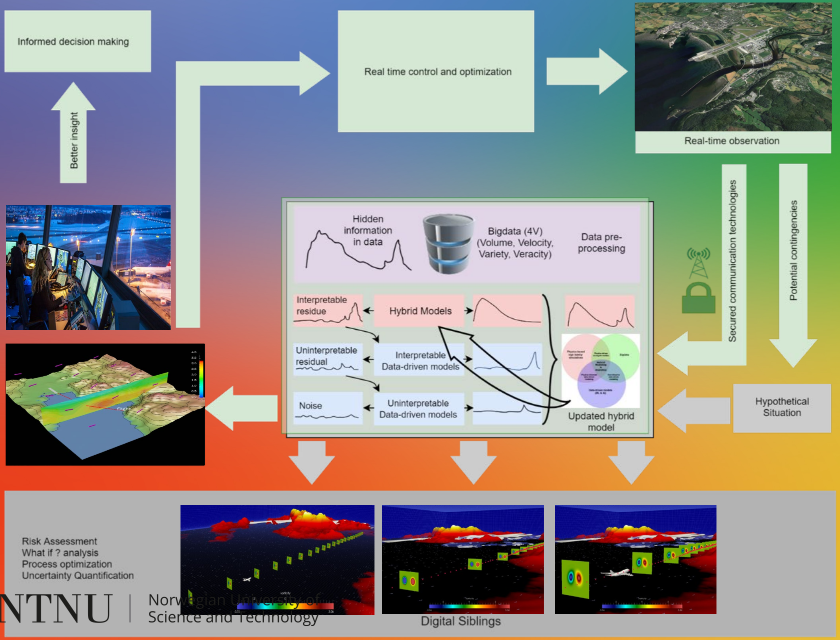
www.hybridmodelling.com

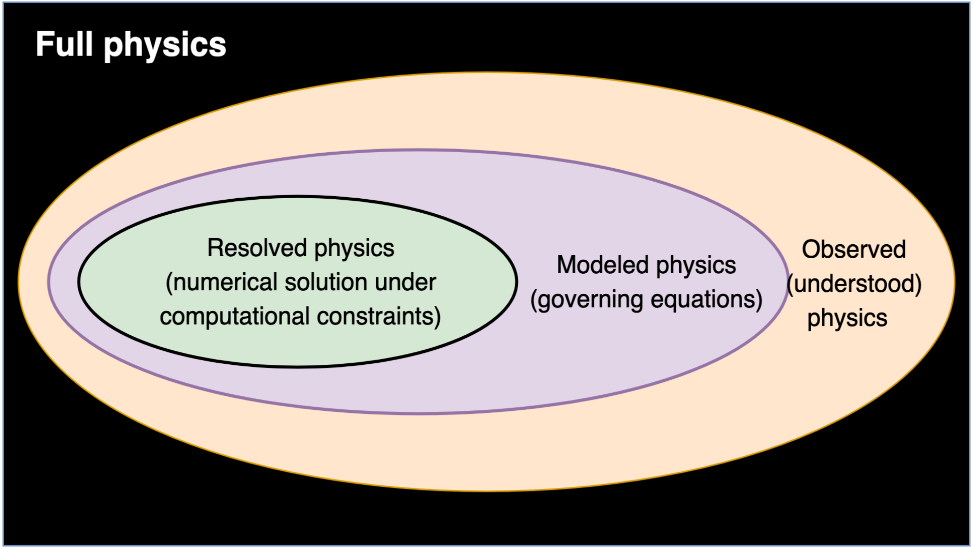
# DIGITAL TWIN

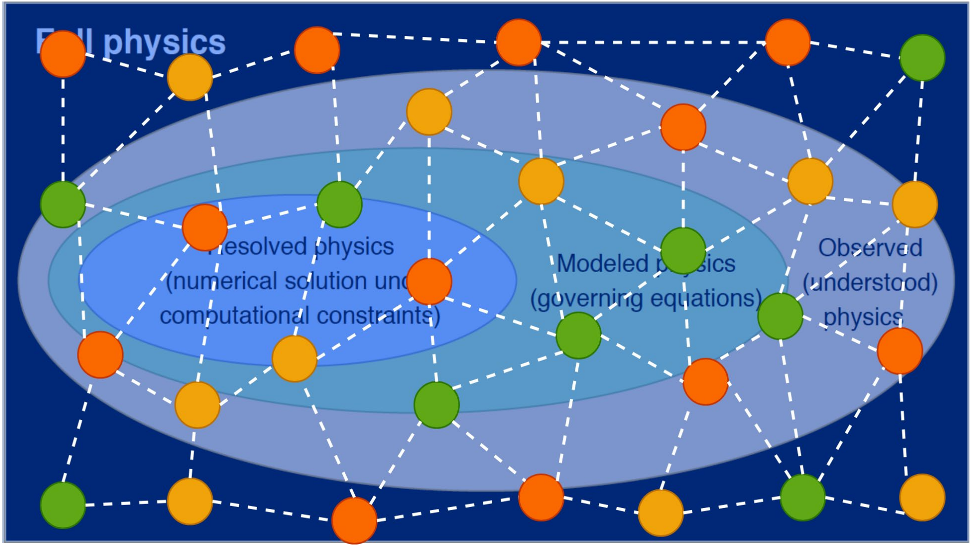



*A **digital twin** is defined as a virtual representation of a physical asset enabled through data and simulators for real-time prediction, monitoring, control and optimization of the asset for improved decision making throughout the life cycle of the asset and beyond.*

# Content - Models are needed

- Physics based modeling (PBM)
- Data-driven modeling (DDM)
- Hybrid / Meta modeling (MM)


Full physics
Resolved physics
(numerical solution under
computational constraints)
Modeled physics
(governing equations)
Observed
(understood)
physics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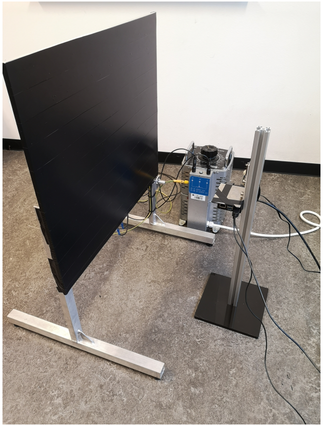
(numerical solution un
computational constraints)
Modeled
(governing equations)
Observed
(understood)
physics

# Content - Example problem



Challenges: How to model the dynamics ?

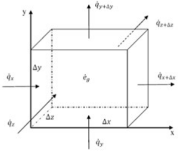
# PBM: - Physics-driven equation discovery

## Modeling

$$\dot{q}_{x+dx} = \dot{q}_x + \frac{\partial \dot{q}_x}{\partial x}\,dx$$

or,

$$\dot{q}_x - \dot{q}_{x+dx} = -\frac{\partial \dot{q}_x}{\partial x}\,dx$$



Fourier's law of heat conduction

$$\dot{q}_x = -k\,dy\,dz\,\frac{\partial T}{\partial x}$$

$$\boxed{\dot{q}_x - \dot{q}_{x+dx} = \frac{\partial}{\partial x}\left(k\,\frac{\partial T}{\partial x}\right) dx\,dy\,dz}$$

$$\dot{q}_y - \dot{q}_{y+dy} = \frac{\partial}{\partial y}\left(k\,\frac{\partial T}{\partial y}\right) dx\,dy\,dz$$

and,

$$\dot{q}_z - \dot{q}_{z+dz} = \frac{\partial}{\partial z}\left(k\,\frac{\partial T}{\partial z}\right) dx\,dy\,dz$$

$$\boxed{\begin{aligned} &\textit{Rate of heat input} + \textit{Rate of heat generation}\\ &\qquad = \textit{Rate of heat output}\\ &\qquad + \textit{Rate of change of heat energy within the body}\end{aligned}}$$

$$\dot{u} = (\rho dx\,dy\,dz)c_p\left(\frac{\partial T}{\partial t}\right)$$

$$(\dot{q}_x + \dot{q}_y + \dot{q}_z) + (\dot{e}_g\,dx\,dy\,dz) = (\dot{q}_{x+dx} + \dot{q}_{y+dy} + \dot{q}_{z+dz}) + (\rho dx\,dy\,dz)c_p\left(\frac{\partial T}{\partial t}\right)$$

$$(\dot{q}_x - \dot{q}_{x+dx}) + (\dot{q}_y - \dot{q}_{y+dy}) + (\dot{q}_z - \dot{q}_{z+dz}) + (\dot{e}_g dx\,dy\,dz) = (\rho dx\,dy\,dz)c_p\left(\frac{\partial T}{\partial t}\right)$$

or,

$$\left\{\frac{\partial}{\partial x}\left(k\,\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\,\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k\,\frac{\partial T}{\partial z}\right)\right\}(dx\,dy\,dz) + (\dot{e}_g\,dx\,dy\,dz) = (\rho dx\,dy\,dz)c_p\left(\frac{\partial T}{\partial t}\right)$$

or,

$$\left\{\frac{\partial}{\partial x}\left(k\,\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\,\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k\,\frac{\partial T}{\partial z}\right)\right\} + \dot{e}_g = \rho c_p\left(\frac{\partial T}{\partial t}\right)$$

# DDM: Data-driven equation discovery - Prerequisite

- Sequential threshold ridge regression (STRidge)
- Least absolute selection operator (LASSO)
- Computation of derivatives numerically

# DDM: Data-driven equation discovery - $L_1$ Regularization: Ridge

$$J(\beta) = \sum_{i=1}^{n}(y_i - \beta_o - \sum_{j=1}^{p}\beta_j x_{ij})^2 + \lambda\sum_{j=1}^{p}\beta_j^2$$

# DDM: Data-driven equation discovery - $L_2$ Regularization: LASSO

$$J(\beta) = \sum_{i=1}^{n}(y_i - \beta_o - \sum_{j=1}^{p} \beta_j x_{ij})^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

# DDM: Data-driven equation discovery - Taylor Series expansion

$$u_{i+1} = u_i + \Delta x \frac{\partial u}{\partial x}|_i + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}|_i + \frac{\Delta x^3}{3}\frac{\partial^3 u}{\partial x^3}|_i + O(\Delta x^4)$$

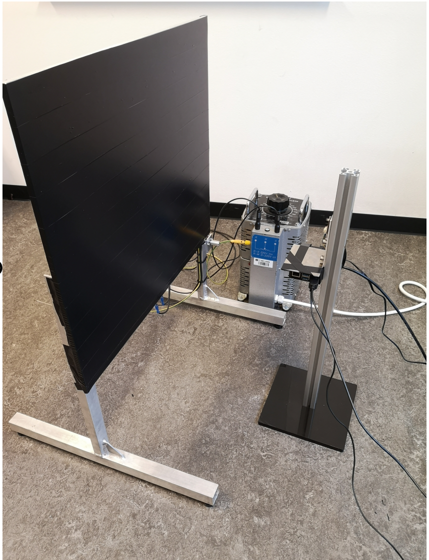
$$u_{i-1} = u_i - \Delta x \frac{\partial u}{\partial x}|_i + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}|_i - \frac{\Delta x^3}{3}\frac{\partial^3 u}{\partial x^3}|_i + O(\Delta x^4)$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + O(\Delta x^2)$$

$$\frac{\partial u}{\partial x} = \frac{u_i^{n+1} - u_i^n}{\Delta t}$$

# DDM: Data-driven equation discovery - Data sampling

$$\mathbf{u} = \left.\overbrace{\begin{bmatrix} u_1(t_1) & u_2(t_1) & \dots & u_n(t_1) \\ u_1(t_2) & u_2(t_2) & \dots & u_n(t_2) \\ \vdots & \vdots & \ddots & \vdots \\ u_1(t_m) & u_2(t_m) & \dots & u_n(t_m) \end{bmatrix}}^{\text{spatial locations}}\right\} \text{time snap} \tag{1}$$



# DDM: Data-driven equation discovery - Feature Engineering

$$u_t = \frac{u_j^{n+1} - u_j^{n-1}}{2dt}$$

$$u_{2t} = \frac{u_j^{n+1} - 2u_j^n + u_j^{n-1}}{dt^2}$$

$$u_x = \frac{u_{j+1}^n - u_{j-1}^n}{2dx}$$

$$u_{2x} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{dx^2}$$

$$u_{3x} = \frac{u_{j+2}^n - 2u_{j+1}^n + 2u_{j-1}^n - u_{j-2}^n}{2dx^3}$$

$$u_{4x} = \frac{u_{j+2}^n - 4u_{j+1}^n + 6u_j^n + -4u_{j-1}^n - u_{j-2}^n}{dx^4}$$

$$u_{5x} = \frac{u_{j+3}^n - 4u_{j+2}^n + 5u_{j+1}^n - 5u_{j-1}^n + 4u_{j-2}^n - u_{j-3}^n}{2dx^5}$$

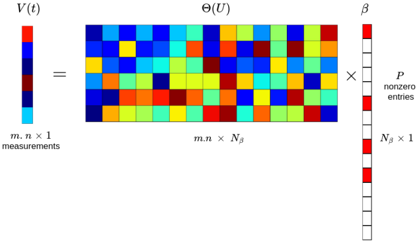
# DDM: Data-driven equation discovery - LASSO regression

$$\mathbf{V(t)} = [\mathbf{U}_t]$$

$$\tilde{\mathbf{\Theta}}(\mathbf{U}) = [\mathbf{U} \quad \mathbf{U}_x \quad \mathbf{U}_{2x} \quad \mathbf{U}_{3x} \quad \mathbf{U}_{4x} \quad \mathbf{U}_{5x}]$$

# DDM: Data-driven equation discovery - Methodology for more complex equations

$$\frac{\partial T}{\partial t} = \nu \left\{ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right\} + S$$



# DDM: Data-driven equation discovery - Numerical Discretization 2D

$$\frac{\partial T}{\partial t} = \nu \left\{ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right\}$$

$$\frac{T_{i,j}^{n+1} - T_{i,j}^{n}}{\Delta t} = \nu \frac{T_{i+1,j}^{n} - 2T_{i,j}^{n} + T_{i-1,j}^{n}}{\Delta x^2} + \nu \frac{T_{i,j+1}^{n} - 2T_{i,j}^{n} + T_{i,j-1}^{n}}{\Delta y^2}$$

$$T_{i,j}^{n+1} = T_{i,j}^{n} + \frac{\nu \Delta t}{\Delta x^2}(T_{i+1,j}^{n} - 2T_{i,j}^{n} + T_{i-1,j}^{n}) + \frac{\nu \Delta t}{\Delta y^2}(T_{i,j+1}^{n} - 2T_{i,j}^{n} + T_{i,j-1}^{n})$$

# MM / HAM - PBM vs DDM

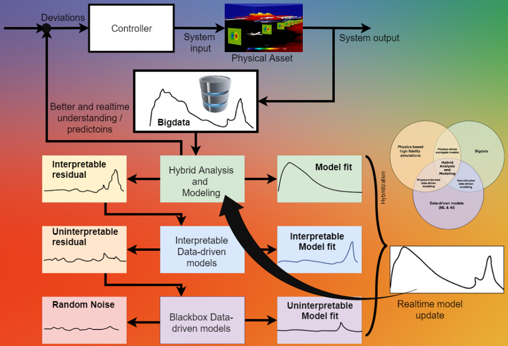
| PBM | DDM |
|---|---|
| +Solid foundation | − Mostly black-boxes |
| − Difficult to assimilate very long term historical data | + Takes into account long term historical data and experiences |
| − Computationally expensive, sensitive and susceptible to numerical instability | + Once the model is trained, it is very stable and efficient for making predictions / inferences |
| + Errors / uncertainties can be bounded and estimated | − Not possible to bound errors / uncertainties |
| + Less susceptible to bias | − Bias in data is reflected in the model prediction |
| + Generalizes well to new problems with similar physics | − Poor generalization on unseen problems |

# MM / HAM - Desired characteristics in a modeling approach

- Generalizability / Robustness
- Trustworthiness / Transparent / Explainable
- Computational efficiency yet accurate
- Dynamically adapting and evolving
- Automated physics discovery

# MM / HAM - Big Data Cybernetics philosophy

## Big Data Cybernetics

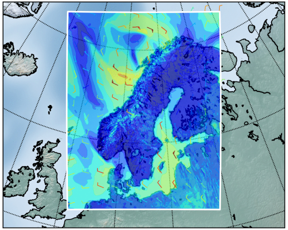


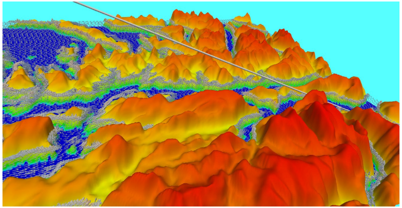

*A new paradigm in steering the world with big data characterized by high volume, high velocity, high vareity and high veracity*

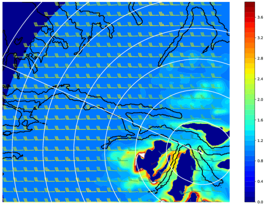
# MM / HAM - What and why ?

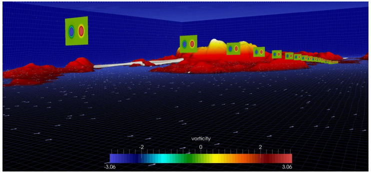
- Metamodeling is a simplified model created from a complex model
- The aim of metamodeling is to invest computational resources to develop fast mathematical approximations of sophisticated, computationally demanding models

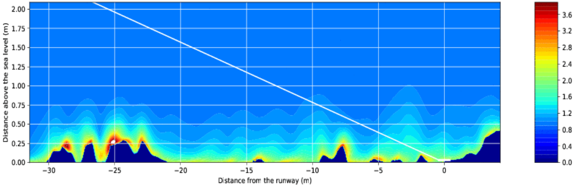
# Aircraft wake modeling



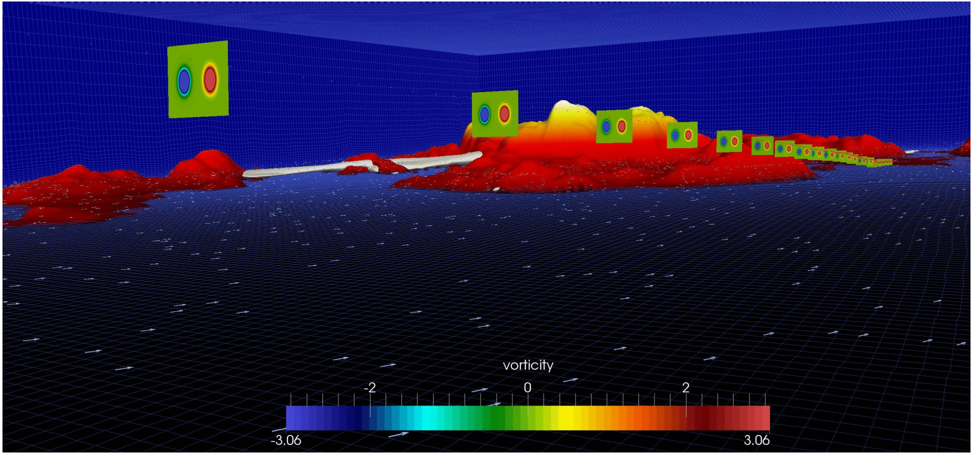




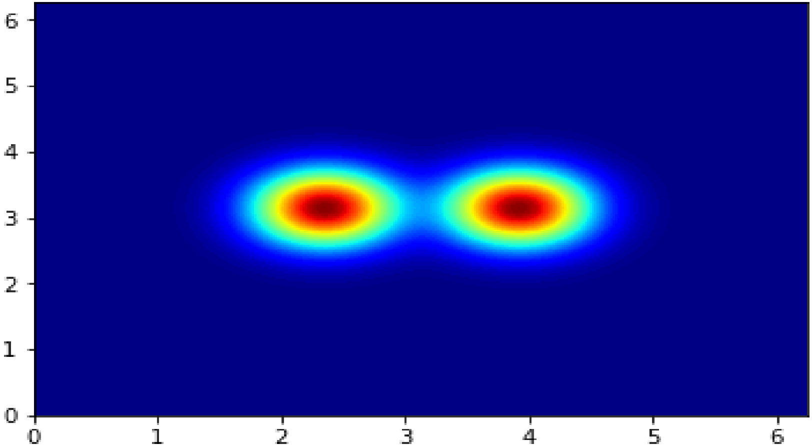


# MM / HAM - Motivation



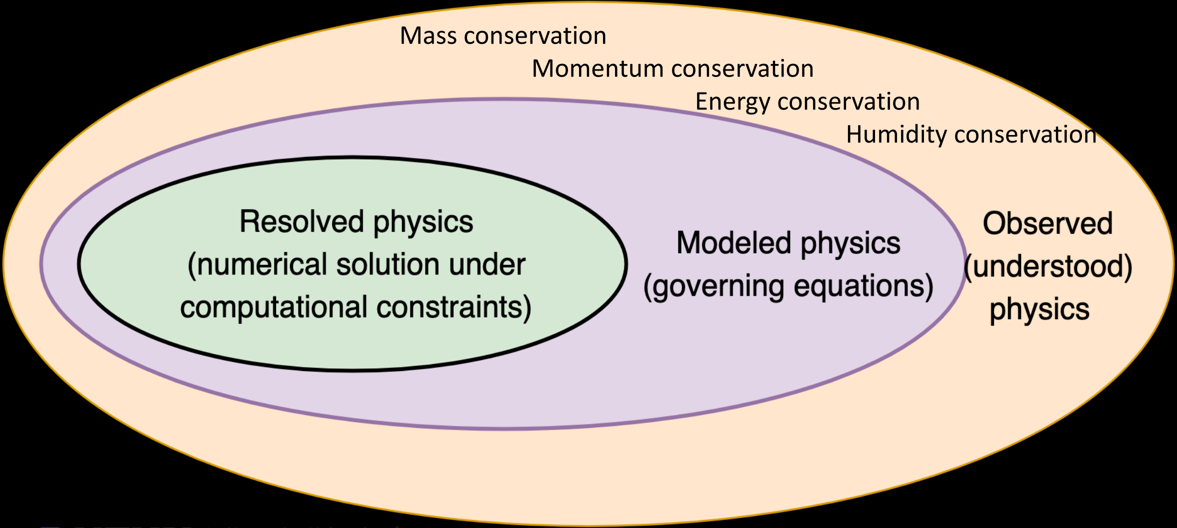
# MM / HAM - Aircraft wakes



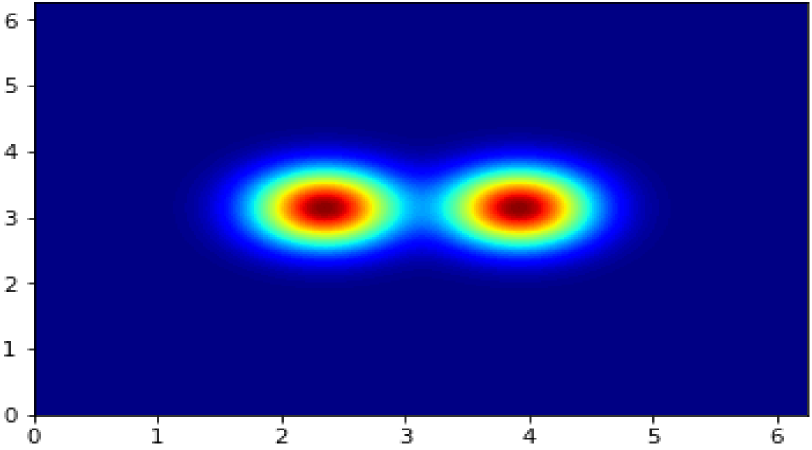
# MM / HAM - Step 1a: Physics based equation discovery

- Mass conservation equation
- Momentum conservation equation
- Energy conservation equation
- Humidity conservation equation
- Unknown physics

# Full physics



# MM / HAM - Step 1b: Data-driven equation discovery



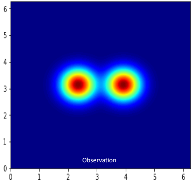
# MM / HAM - Discovered equation

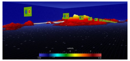
$$\frac{\partial \omega}{\partial t} + \frac{\partial \psi}{\partial y}\frac{\partial \omega}{\partial x} - \frac{\partial \psi}{\partial x}\frac{\partial \omega}{\partial y} = \frac{1}{\mathrm{Re}}\left(\frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2}\right) + \Pi$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = -\omega$$

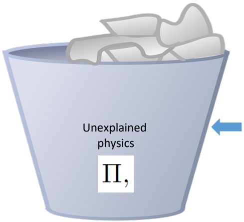
where $\omega$ is the vorticity defined as $\omega = \nabla \times u$, $u = [u, v]^T$ is the velocity vector, and $\psi$ is the stream function

# MM / HAM - Step 1: Physics based modeling



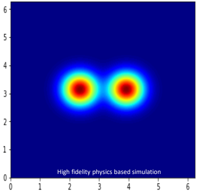
Snapshots using LIDARS and RADARS




$$\frac{\partial \omega}{\partial t} + J(\omega, \psi) = \frac{1}{Re}\nabla^2 \omega$$

$$J(\omega, \psi) = \frac{\partial \psi}{\partial y}\frac{\partial \omega}{\partial x} - \frac{\partial \psi}{\partial x}\frac{\partial \omega}{\partial y} \qquad \nabla^2 \psi = -\omega$$

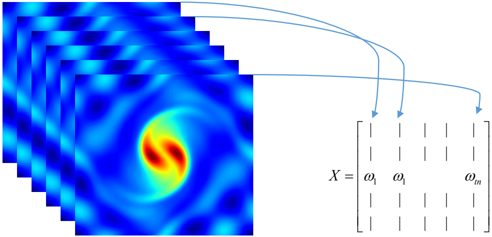
Generalization

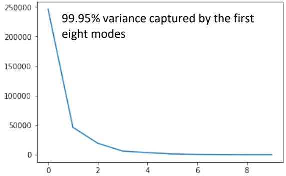


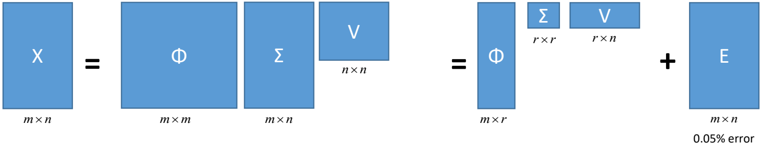

☺ Better Generalization
☹ Computationally expensive
☹ Inaccurate

Python notebook

# MM / HAM - Step 2: PCA: Computing the principal components

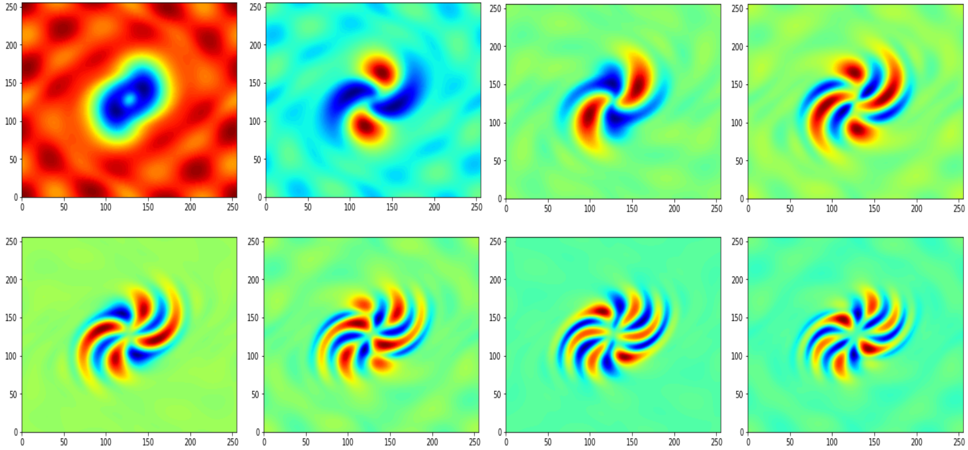



Python notebook

# MM / HAM - Orthonormal basis for a particular Reynolds Number



# MM / HAM - Different basis for different Reynolds Number

# MM / HAM - Step 3: Galerkin projection / dimensionality reduction

$$\frac{\partial \omega}{\partial t} + \frac{\partial \psi}{\partial y}\frac{\partial \omega}{\partial x} - \frac{\partial \psi}{\partial x}\frac{\partial \omega}{\partial y} = \frac{1}{\mathrm{Re}}\left(\frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2}\right) + \Pi$$

# MM / HAM - Step 3: Galerkin projection / dimensionality reduction

$$\frac{\partial \omega}{\partial t} + \frac{\partial \psi}{\partial y}\frac{\partial \omega}{\partial x} - \frac{\partial \psi}{\partial x}\frac{\partial \omega}{\partial y} = \frac{1}{\mathrm{Re}}\left(\frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2}\right) + \Pi$$

$$\omega\left(x, t_n\right) = \sum_{k=1}^{R} a_k(t_n)\phi_k(x)$$

# MM / HAM - Step 3: Galerkin projection / dimensionality reduction

$$\frac{\partial \omega}{\partial t} + \frac{\partial \psi}{\partial y}\frac{\partial \omega}{\partial x} - \frac{\partial \psi}{\partial x}\frac{\partial \omega}{\partial y} = \frac{1}{\mathrm{Re}}\left(\frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2}\right) + \Pi$$

$$\omega\left(x, t_n\right) = \sum_{k=1}^{R} a_k(t_n)\phi_k(x)$$

$$\frac{\mathrm{d}a_k}{\mathrm{d}t} = \underbrace{\sum_{i=1}^{R} \mathfrak{L}_{ik} a_i + \sum_{i=1}^{R}\sum_{j=1}^{R} \mathfrak{N}_{ijk} a_i a_j}_{\text{Physics-based model } G(a_k)} + \underbrace{\tilde{C}_k}_{\text{Hidden physics}}$$

# MM / HAM - Step 3: Galerkin projection / dimensionality reduction

$$\frac{\mathrm{d}a_k}{\mathrm{d}t} = \underbrace{\sum_{i=1}^{R} \mathfrak{L}_{ik} a_i + \sum_{i=1}^{R}\sum_{j=1}^{R} \mathfrak{N}_{ijk} a_i a_j}_{\text{Physics-based model } G(a_k)} + \underbrace{\tilde{C}_k}_{\text{Hidden physics}}$$

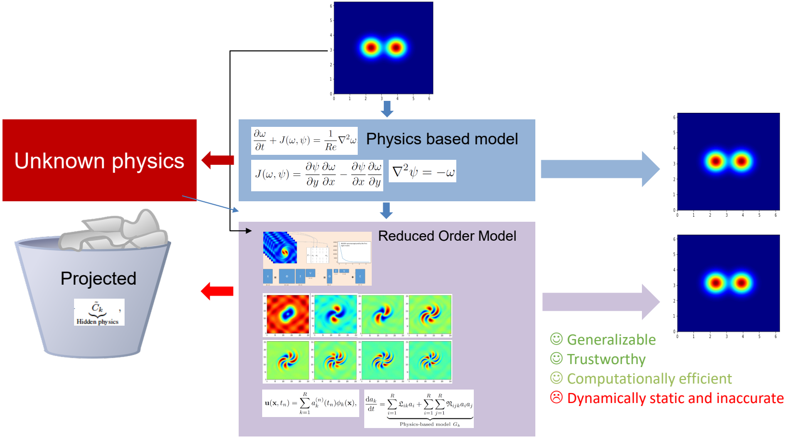
where

$$\mathfrak{L}_{ik} = \left\langle \frac{1}{\mathrm{Re}} \left( \frac{\partial^2 \phi_i^\omega}{\partial x^2} + \frac{\partial^2 \phi_i^\omega}{\partial y^2} \right), \phi_k^\omega \right\rangle$$

$$\mathfrak{N}_{ijk} = \left\langle -\left( \frac{\partial \phi_i^\omega}{\partial x}\frac{\partial \phi_j^\psi}{\partial y} - \frac{\partial \phi_i^\omega}{\partial y}\frac{\partial \phi_j^\psi}{\partial x} \right), \phi_k^\omega \right\rangle$$

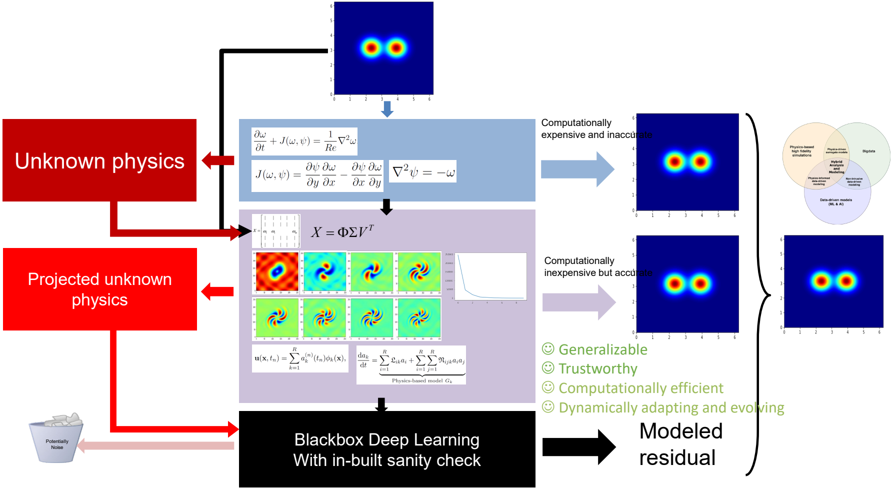
Python notebook

# MM / HAM – Results using GP-ROM

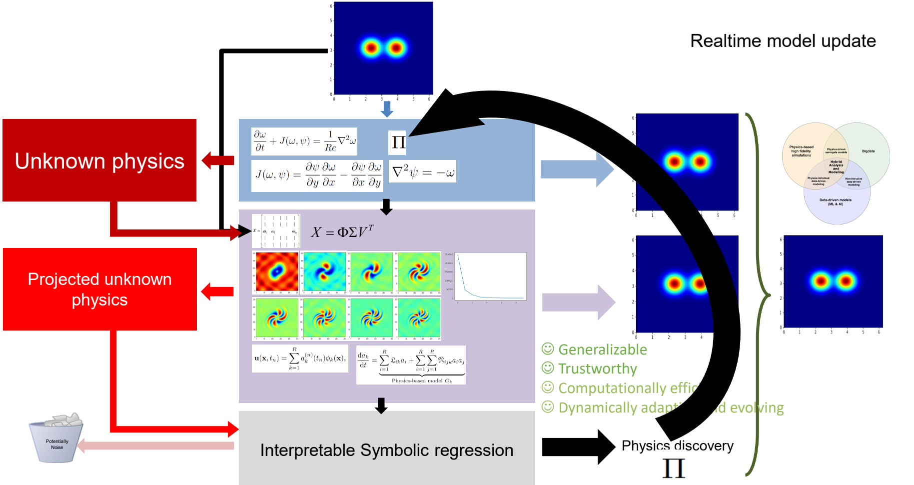



- ☺ Generalizable
- ☺ Trustworthy
- ☺ Computationally efficient
- ☹ Dynamically static and inaccurate

# MM / HAM – DL-based correction

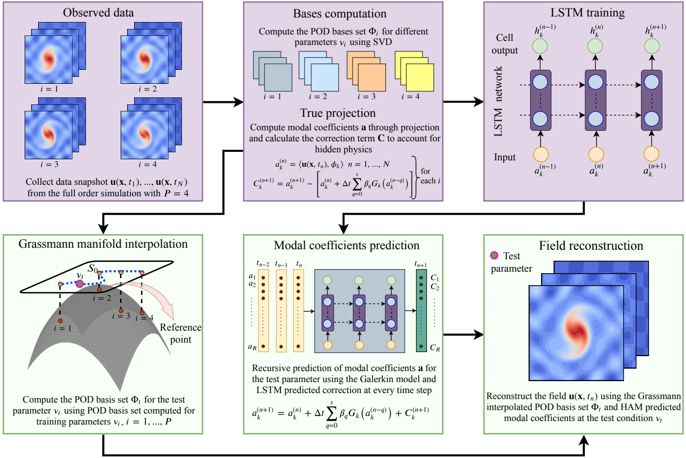


# MM / HAM - Model update




$$= 0.0099\ \sin(x)\ \cos(y)\ \exp(-0.078\ t) - 1.47 \times 10^{-6}$$

# MM / HAM – Full algorithm



Thank you for your attention

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